Behavior of the two-dimensional Ising model at the boundary of a half-infinite cylinder

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Abstract

The two-dimensional Ising model is studied at the boundary of a half-infinite cylinder. The three regular lattices (square, triangular and hexagonal) and the three regimes (sub-, super- and critical) are discussed. The probability of having precisely $2n$ spinflips at the boundary is computed as a function of the positions k_i's, $i = 1, \ldots, 2n$, of the spinflips. The limit when the mesh goes to zero is obtained. For the square lattice, the probability of having $2n$ spinflips, independently of their position, is also computed. As a byproduct we recover a result of De Coninck showing that the limiting distribution of the number of spinflips is Gaussian. The results are obtained as consequences of Onsager's solution and are rigorous.

1 Introduction

The present paper gives a rigorous description of the spin configurations seen at the end of a half-infinite cylinder covered by the Ising model on square, triangular or hexagonal lattices. Both the discrete case and its continuous limit are made explicit. Section 2, devoted to the square lattice, describes the boundary behavior by giving, for a fixed number $2n$ of spinflips, the probability distribution as a function of the positions of the spinflips. The three regimes, subcritical, critical and supercritical, are discussed. It should be stressed that these probabilities *are not* correlation functions, even though they can be used to calculate them. In Section 3 we compute, for the square lattice, the distribution of the random variable (number of spinflips) / (number of sites at the boundary) at the critical temperature. Section 4 extends the results of Section 1 to the triangular and hexagonal lattices. The results (and the methods to obtain them) are simple, though non-trivial, and the thermodynamical limits are shown to depend only on the behavior of smooth functions defined on $[-\pi, \pi]$ for the

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square lattice and on $[-\pi/2, \pi/2]$ for the other two. Only their behavior at zero and at the extremities on these intervals play a role.

The calculation presented here could have been done by several methods and for other orientations of the lattices. We chose the most classical technique, the one based on the transfer matrix; in the present case, this method turns out to be simple and scientists with expertise in neighboring fields will be able to follow the argument with minimal investment. It is impossible to make a short overview of more than sixty years of developments on the Ising model. There are two results however that we emphasize since they are directly related to ours. Abraham [1] proved that the limit distribution, with a non-trivial scaling, for the magnetization of the Ising model on a square lattice is Gaussian at the edge of a half-infinite cylinder and at criticality. Along the same line, De Coninck [6] showed that in the limit the joint distribution for the magnetization and the energy (which is a linear function of the number of spinflips) is also Gaussian. The two proofs use the transfer matrix method to directly compute the characteristic function of the variables. We recover here De Coninck's result for the number of spinflips using the distribution in the discrete case computed in Section 2 and a combinatorial lemma found in the Appendix. We obtain explicit expressions for both the mean and the variance of the limiting distribution.

Finding the relative weights of boundary configurations as a function of the number and locations of spinflips might seem only a mildly interesting exercise. A word of explanation is therefore in order. With the invention of the stochastic Loewner equation (SLE) by Schramm [19] and proofs by Smirnov [21] that percolation and the Ising model are conformally invariant in the limit when the mesh goes to zero, new rigorous tools have been available to probe critical phenomena, and with these tools, new observables have been introduced. Suppose that boundary conditions are imposed at the extremity of the half-infinite cylinder as follows. Let $0 \le \theta_1 < \theta_2 < \theta_3 < \theta_4 < 2\pi$ be four angles. They define four intervals along the boundary and we suppose that the sign of Ising spins are constant on each, but alternate from one interval to the next. Such boundary conditions force interfaces, that is contours between constant-sign clusters, to intersect the boundary at the θ's, and only there. Since these interfaces cannot cross, the interface starting at θ_1 must end at θ_2 or θ_4. One can therefore ask what is the probability that the interface starting at θ_1 goes to θ_2. At least five groups in the last eight years computed this new "observable", and they all had to solve the problem that is the subject of the present paper. The first two groups, two of the present authors [2], and Bauer, Bernard and Kytölä [3], used conformal field theory (CFT) to do it, even though the latter group was actually interested in devising a way to define multiple SLE processes. The three other groups used purely SLE methods to obtain the result [20, 8, 9]. We were not able to compute directly from the lattice models the probability just described. This is why we turned in [2] to CFT to do it. And this is why the present paper limits itself to computing the relative weights as functions of the number and locations of spinflips, disregarding how the interfaces join the spinflips. Despite its limitations, the calculation has several redeeming features. First, it is done from first principles and relies on classical methods. Second, contrarily to the results obtained from SLE or CFT, it gives an explicit result for any number of spinflips, not only for four. Third, it allows for subcritical and supercritical regimes to be studied. Finally, it provides information on a mesoscopic scale, namely on the distribution of the number of spinflips at the boundary. We note also that

the continuous distribution for the positions of four spinflips at the boundary (cf. equation (15)) was an important element in the computation just described [2].

2 Behavior at the boundary for the square lattice

2.1 Notation

Let $\sigma : \{1, 2, \dots, m\} \to \{+1, -1\}$ be a configuration along the circular extremity of a half-infinite cylinder covered by the square lattice. The number m of sites on this circle is taken to be even. It is convenient to encapsulate the information contained in σ in the following data: the value $s \in \{+1, -1\}$ of σ at 1 and the positions $k_i \in \{1, 2, \dots, m\}, 1 \le i \le 2n$, of spinflips. A spinflip in σ occurs at k_i if $\sigma_{k_i-1} = -\sigma_{k_i}$ with $\sigma_0 = \sigma_m$ and $\sigma_1 = \sigma_{m+1}$ by definition. We choose $1 \le k_1 < k_2 < ... < k_{2n} \le m$. The number n can also be seen as the number of maximally connected stretches of $+$-spins along the boundary. We identify the functions σ with their data $(s; k_1, k_2, \dots, k_{2n})$.

If σ and σ' are two configurations on contiguous circles along the cylinder, the transfer matrix $T : \mathbb{C}^{2^m} \to \mathbb{C}^{2^m}$ is given by its matrix elements $T_{\sigma;\sigma'} = \exp(\nu \sum_{k=1}^m \sigma_k \sigma_{k+1} + \nu \sum_{k=1}^m \sigma_k \sigma'_k)$. The constant ν is the product of the coupling constant of the Ising model taken here to be isotropic, with the inverse temperature measured in units that make the Boltzmann constant unity. We shall refer to ν as the inverse temperature. The critical temperature is defined by $\sinh 2\nu_c = 1$. When the Ising model is on a torus, there is some freedom in the choice of the transfer matrix. Here this choice is unique as the transfer matrix must include the Boltzmann weights attached to the bonds between the m sites at the boundary and the bonds that tie them to the first inner circle.

Note that all matrix elements are positive. By Perron-Frobenius theorem, the transfer matrix has real eigenvalues. Moreover its largest eigenvalue is non-degenerate. Let ω be a non-zero eigenvector corresponding to this eigenvalue and let $c^s(k_1, k_2, \dots, k_{2n})$ be its components in the state basis. It is known that these components can be chosen such that they are all positive and that their sum is 1. With this choice, the probability of a given state σ

$$\Pr(\sigma = (s; k_1, k_2, \dots, k_{2n})) = c^s(k_1, k_2, \dots, k_{2n})/\kappa \tag{1}$$

where

$$\kappa = \sum_{s \in \{+1,-1\}} \sum_{n=0}^{m/2} \sum_{1 \le k_1 < k_2 < \dots < k_{2n} \le m} c^s(k_1, k_2, \dots, k_{2n}).$$

Note that the $c^s(k_1, k_2, \dots, k_{2n})$'s do not depend on s and this super-index will be deleted when it is appropriate.

We use Thompson's notation [18] in the rewriting of T in terms of tensorial blocks. The Pauli matrices $\tau^1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right), \tau^2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \tau^3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, and $\mathbf{1} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ are used to define $2^m \times 2^m$-matrices $\tau_k^i = \mathbf{1} \otimes \cdots \otimes \tau^i \otimes \cdots \otimes \mathbf{1}, i \in \{1, 2, 3\}$ and $1 \le k \le m$, where the only non-trivial factor is at position k. The following operators ($\mathbb{C}^{2^m} \to \mathbb{C}^{2^m}$) will also be used: $\rho_k = \tau_1^1 \tau_2^1 \dots \tau_{k-1}^1 \tau_k^2$, and $\pi_k = \tau_1^1 \tau_2^1 \dots \tau_{k-1}^1 \tau_k^3$ where again $k \in \{1, 2, \dots, m\}$. The linear combinations $a_k = \frac{1}{2}(\rho_k + i\pi_k)$ and $a_k^\dagger = \frac{1}{2}(\rho_k - i\pi_k)$, $k \in \{1, 2, \dots, m\}$, satisfy

$a_k a_{k'}^\dagger + a_{k'}^\dagger a_k = \delta_{kk'} \mathbf{1}_{2^m}$ and $a_k a_{k'} + a_{k'} a_k = \mathbf{0}_{2^m}$. Finally their Fourier coefficients are given by

$$\eta_q = \frac{e^{-i\pi/4}}{\sqrt{m}} \sum_{1\le k\le m} e^{-iqk} a_k \qquad \text{and} \qquad \eta_q^\dagger = \frac{e^{i\pi/4}}{\sqrt{m}} \sum_{1\le k\le m} e^{iqk} a_k^\dagger$$

for $q \in Q_m$, the set of phases of the m-roots of -1: $Q_m = \left\{\frac{(2j-1)\pi}{m}, -\frac{m}{2}+1 \le j \le \frac{m}{2}\right\}$. Using this notation, the transfer matrix is

$$T = (2\text{sinh}2\nu)^{\frac{m}{2}} \exp(i\nu\pi_1\rho_m P) \exp\left(-i\nu \sum_{1\le k\le m-1} \pi_{k+1}\rho_k\right) \exp\left(i\nu^* \sum_{1\le k\le m} \pi_k\rho_k\right)$$

where $P = \prod_{1\le k\le m} \tau_k^1$, $P^2 = \mathbf{1}_{2^m}$, is the operator flipping a configuration $\sigma = (s; k_i)$ into $(-s; k_i)$ and ν^* is defined implicitly by $\sinh 2\nu \sinh 2\nu^* = 1$. Since the Boltzmann weights are invariant under the flip of all spins, P commutes with the transfer matrix and T and P can be diagonalized simultaneously. The eigenvector ω belongs to the $+$-eigensubspace of P.

The eigenvectors of T are constructed with creation and annihilation operators $\xi_q^\dagger$ and $\xi_q, q \in Q_m$, obtained from the η_q and $\eta_q^\dagger$ by orthogonal transformations. They are $\xi_q = \eta_q \cos\phi_q + \eta_{-q}^\dagger \sin\phi_q$ and $\xi_{-q} = \eta_{-q}\cos\phi_q - \eta_q^\dagger \sin\phi_q$ with

$$\tan\phi_q = \frac{(\tanh 2\nu + \sinh 2\nu)\sin q}{1 - 2\sinh 2\nu \cos q + \sqrt{(\cosh 2\nu - \tanh 2\nu(\cos q + 1))(\cosh 2\nu - \tanh 2\nu(\cos q - 1))}}.$$

Though our choice of the transfer matrix, and therefore our expression for $\tan\phi_q$, are different from those used in [22], the reader will find in that reference the method to obtain this expression. The eigenspace spanned by ω is characterized algebraically as the one-dimensional kernel of the m operators ξ_q:

$$\xi_q \omega = 0, \qquad q \in Q_m. \tag{2}$$

The other eigenstates of T in the maximal subspace $V_+ \subset V$ where $P|_{V_+} = 1$ are obtained by acting with an even number of $\xi_q^\dagger$ on the vacuum ω. Because the ξ_q and $\xi_{q'}^\dagger$ anticommute like the pairs $a_k, a_{k'}^\dagger$'s and $\eta_q, \eta_{q'}^\dagger$'s, a vector $\xi_{q_1}^\dagger \xi_{q_2}^\dagger \dots \xi_{q_{2i}}^\dagger \omega$ is a non-zero eigenstate only if the q_i's are distinct. Equation (2) is the one to be solved.

2.2 The discrete and continuous cases $n = 1$

Suppose σ describes a configuration with a single stretch of $-$-spins and a single stretch of $+$-spins. Then $\sigma = (s; k_1, k_2)$ and $n = 1$. This paragraph is devoted to computing $\Pr(\sigma = (s; k_1, k_2))$ in the discrete case, cf. equation (3), and in the limit, cf. Proposition 3.

By translation invariance, it is sufficient to compute $c^+(1, k)$. The operators τ_k^1 flip the spin at position k and the operators ρ_k and π_{k+1} flip all the spins from 1 to k inclusively. The operators ξ_q are linear combinations of these and the component along $\sigma_\uparrow$ (the configuration with only $+$-spins) in $\xi_q\omega$ can therefore originate only from the action of ξ_q on $\sigma_\uparrow$ or on a

σ of the form $(-;1,k)$. If we denote by $(u)_v$ the component along v in the vector u (in the basis given by the σ's), then

$$(\eta_q\omega)_{\sigma_\uparrow} = \frac{ie^{-i\pi/4}}{2\sqrt{m}}\left(e^{-iq}c_\uparrow - e^{-iqm}c_\downarrow + \sum_{2\le k\le m} e^{-iqk}c^-(1,k)(1-e^{iq})\right)$$

and

$$(\eta^\dagger_{-q}\omega)_{\sigma_\uparrow} = \frac{-ie^{i\pi/4}}{2\sqrt{m}}\left(e^{-iq}c_\uparrow + e^{-iqm}c_\downarrow + \sum_{2\le k\le m} e^{-iqk}c^-(1,k)(1+e^{iq})\right)$$

Using $c_\uparrow = c_\downarrow$ and $e^{iqm}=-1$ for $q\in Q_m$, the vanishing of $(\xi_q\omega)_{\sigma_\uparrow}$ gives $i\sum_{2\le k\le m} e^{-iq(k-1)}c^-(1,k) = c_\uparrow \cot(\phi_q+\frac{q}{2})$. Using the discrete inverse Fourier transform and translation symmetry, one gets:

$$c^s(k_1,k_2) = -\frac{ic_\uparrow}{m}\sum_{q\in Q_m} e^{iq(k_2-k_1)}\cot(\phi_q+\tfrac{q}{2}). \tag{3}$$

That $c^s(k_1,k_2)$ is a real number follows from $c^\pm(1,k)=c^\pm(1,m+2-k)$ and the fact that ϕ_q is an odd function of q. The expression for $\cot(\phi_q+\frac{q}{2})$ is surprisingly similar to that of $\tan\phi_q$:

$$\begin{aligned} d(\nu,q) &= \cot(\phi_q+\tfrac{q}{2}) \\ &= \frac{(1-\tanh 2\nu)\sin q}{\sinh 2\nu - \cos q + \sqrt{(\cosh 2\nu - \tanh 2\nu(\cos q+1))(\cosh 2\nu-\tanh 2\nu(\cos q - 1))}}. \end{aligned} \tag{4}$$

We note as a curiosity the following simple relation: $\cot(\phi_q+\frac{q}{2}) = \frac{\sqrt{2}-1}{\sqrt{2}+1}\tan\phi_q$ at $\nu=\nu_c$. We gather in a lemma the elementary properties of $d(\nu,q)$ that are needed for the limit.

Lemma 1 *The function $d:\mathbb{R}^+\times\mathbb{R}\to\mathbb{R}$ defined by $d(\nu,q)=\cot(\phi_q+q/2)$ given above has the following properties:*

(i) *for any $\nu\in(0,\infty)$, d has a simple zero at $q=n\pi$, n odd;*

(ii) *around $q=0$ (or any $q=2n\pi, n\in\mathbb{Z}$), the function has the following behavior*
- $\nu>\nu_c$ *(subcritical)* — $d(\nu,q=0)=0$ *and is smooth around this point*
- $\nu=\nu_c$ *(critical)* — $d(\nu,q)$ *has a jump at* $q=0$ *with* $\sqrt{2}-1=\lim_{q\to0^+}d(\nu_c,q) = -\lim_{q\to0^-}d(\nu_c,q)$
- $\nu<\nu_c$ *(supercritical)* — $d(\nu,q)$ *has a simple pole at* $q=0$;

(iii) *outside the behavior along the lines $q=2n\pi$ stated in* (ii), *$d(\nu,q)$ is analytic in q for all inverse temperatures ν.*

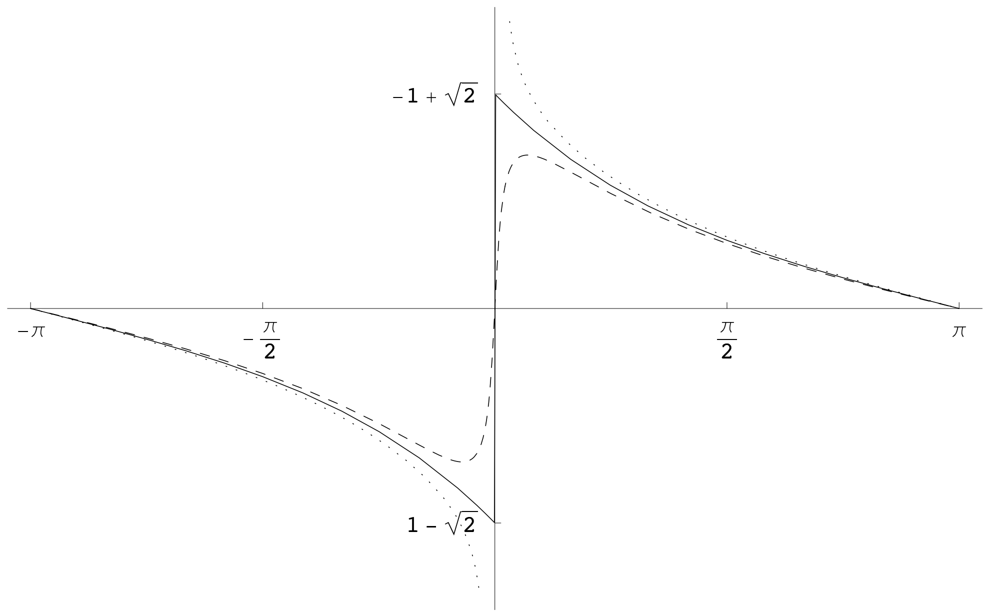

Figure 1: The three regimes of the function $\cot(\phi_q + q/2)$: subcritical (dashed curve), critical (plain curve) and supercritical (dotted curve).

Figure 2.2 draws a graph of these three regimes.

PROOF: Property *(i)* is obtained by direct evaluation. For *(ii)* and *(iii)* note first that the argument of the square root appearing in the denominator vanishes only when $\frac{\cosh 2\nu}{\tanh 2\nu} = \cos q \pm 1$. Because the lhs has a single minimum at $\nu = \nu_c = \frac{1}{2}\text{arcsinh}\, 1$ and is equal to 2, the argument of the square root is zero for $\nu = \nu_c$ and $q \in 2\pi\mathbb{Z}$ only.

For $\nu > \nu_c$, the square root is positive since $\sinh 2\nu > 1 \geq \cos q$, and the denominator never vanishes. The analyticity of the subcritical case follows. For $\nu \leq \nu_c$, the extrema of the argument of the square root can be found to be at $q \in \pi\mathbb{Z}$ with minima at $q = 2n\pi$. The denominator at $q = n\pi, n$ odd, is equal to $1 + \sinh 2\nu + \sqrt{\cosh 2\nu(\cosh 2\nu + 2\tanh 2\nu)}$ and is therefore positive. To check whether it vanishes it is sufficient to evaluate it at its minimum $q = 0$. At this point the denominator is $\sinh 2\nu - 1 + \sqrt{(1 - \sinh 2\nu)^2}$. Since $\sinh 2\nu_c = 1$, we have that the denominator vanishes only when $q = 0$ and $\nu \leq \nu_c$. For $\nu < \nu_c$, the expansion around $q = 0$ of the denominator is $\frac{q^2}{2}(\cosh^2 2\nu(1 - \sinh 2\nu))^{-1} + \mathcal{O}(q^4)$. Because of the $\sin q$ in the numerator, the supercritical behavior described in *(ii)* and *(iii)* is established. For $\nu = \nu_c$, the function d takes the simple form

$$d(\nu_c, q) = \frac{(\sqrt{2} - 1)\sin q}{\sqrt{2}(1 - \cos q) + \sqrt{(1 - \cos q)(3 - \cos q)}}.$$

The leading behavior of its denominator around $q = 0$ is $\sqrt{q^2 + \mathcal{O}(q^4)} + \frac{q^2}{\sqrt{2}} + \mathcal{O}(q^4)$ which accounts for the jump. $\square$

Before turning to the continuum result, we need a technical lemma that rewrites the limit of equation (3) when d is smooth. Equation (3) shows that $c^s(k_1, k_2)$ depends only on the ratio $(k_2 - k_1)/m$ since $iq(k_2 - k_1) = i(2j - 1)\pi(k_2 - k_1)/m$. The meanfingful thing to do is to obtain the limit of that expression when $\frac{\theta}{2\pi} = \frac{k_2 - k_1}{m} \in \mathbb{Q} \cap (0, 1)$ is held fixed. For this fixed ratio, the m's involved in the limit will have to verify two conditions: (1) If $\frac{\theta}{2\pi} \in \mathbb{Q}$ is written as $\frac{p}{n}$ for two relatively prime integers, then n must divide the m's used in the sequence. This ensures that $\frac{\theta}{2\pi}$ is actually of the form $(k_2 - k_1)/m$. The second condition is more technical and its meaning will be clear in Section 4. In the case of the square lattice, the momenta q can be restricted to the interval $[-\pi, \pi]$. For the triangular and hexagonal lattices, they lie in $[-\frac{\pi}{2}, \frac{\pi}{2}]$. We introduce $\gamma \in \mathbb{N}$ such that the momentum range is $[-\frac{2\pi}{\gamma}, \frac{2\pi}{\gamma}]$. The second condition on m's is: (2) $r := \frac{m}{\gamma} \mod n$ is constant.

LEMMA 2 *(i) Let* $z : [0, \frac{2\pi}{\gamma}] \to \mathbb{R}$, $\gamma \in \mathbb{N}$ *be such that* z, z' *and* z'' *exist and are continuous on* $[0, \frac{2\pi}{\gamma}]$. *Let* $\frac{\theta}{2\pi} = \frac{p}{n}$ *with* $\gcd(p, n) = 1$. *Then*

$$\lim_{m\to\infty} 2\sum_{j=1}^{m/\gamma} \sin\left((2j-1)\frac{\theta}{2}\right) z\left((2j-1)\frac{\pi}{m}\right) = \frac{1}{\sin(\theta/2)}\left(z(0) - z(\tfrac{2\pi}{\gamma})\cos(r\theta)\right) \tag{5}$$

$$\lim_{m\to\infty} 2\sum_{j=1}^{m/\gamma} \cos\left((2j-1)\frac{\theta}{2}\right) z\left((2j-1)\frac{\pi}{m}\right) = \frac{\sin(r\theta)}{\sin(\theta/2)} z(\tfrac{2\pi}{\gamma}) \tag{6}$$

where the limits are taken over integer m*'s such that* n *and* γ *divide* m *and such that* $r := m/\gamma \mod n$ *is constant.*
(ii) If $z(\frac{2\pi}{\gamma}) = 0$, *the above results hold without the requirement that* r *be held constant.*

PROOF: *(i)* We divide the range of $j \in \{1, 2, \ldots, \frac{m}{\gamma}\}$ into subsets of n consecutive elements: $\{1, 2, \ldots, n\}, \{n+1, n+2, \ldots, 2n\}$ and so on. There will be r elements left. Omitting these r terms for the present, we consider the sum

$$S_m := \sum_{l=0}^{[\frac{m}{n\gamma}]-1} \sum_{j=0}^{n-1} e^{i(2(j+ln)+1)\theta/2} z((2(j+ln)+1)\pi/m) \;\; = \sum_{l=0}^{[\frac{m}{n\gamma}]-1} \sum_{j=0}^{n-1} e^{i(2j+1)\theta/2} z(q_l + 2j\pi/m) \tag{7}$$

where $q_l = (2ln + 1)\pi/m$ and $[x]$ stands for the integer part of x. By Taylor expansion $z(q_l + 2j\pi/m) = z(q_l) + \frac{2j\pi}{m} z'(q_l) + \frac{4j^2\pi^2}{2m^2}\epsilon_{l,j}$ with $|\epsilon_{l,j}| \le s := \sup_{q\in[0,2\pi/\gamma]} |z''(q)| < \infty$. The two sums $\sum_{j=0}^{n-1} e^{i(2j+1)\theta/2}$ and $\sum_{j=0}^{n-1} j e^{i(2j+1)\theta/2}$ are easily calculated. At $\frac{\theta}{2\pi} = \frac{p}{n}$, the first vanishes and the second is $\frac{n}{2i\sin\theta/2}$. The sum (7) is then

$$\sum_{l=0}^{[\frac{m}{n\gamma}]-1} \sum_{j=0}^{n-1} e^{i(2j+1)\theta/2} \left(z(q_l) + \frac{2j\pi}{m}(z'(q_l) + \epsilon_{l,j})\right)$$
$$= \frac{n\pi}{im}\frac{1}{\sin\theta/2} \sum_{l=0}^{[\frac{m}{n\gamma}]-1} z'(q_l) + \frac{2\pi^2}{m^2} \sum_{l=0}^{[\frac{m}{n\gamma}]-1} \sum_{j=0}^{n-1} j^2 e^{i(2j+1)\theta/2}\epsilon_{l,j}.$$

The second sum goes to zero since its absolute value is smaller than $2\pi^2 n^2 s/\gamma m$. The first sum is a Riemann sum whose limit on m is

$$\lim_{m\to\infty} S_m = \frac{1}{2i\sin\theta/2}\int_0^{2\pi/\gamma} z'(q)dq = \frac{i}{2\sin\theta/2}(z(0) - z(\tfrac{2\pi}{\gamma})). \tag{8}$$

We now turn to the r residual terms: $R_m := \sum_{j=m/\gamma-r+1}^{m/\gamma} e^{i(2j-1)\theta/2} z((2j-1)\pi/m)$. We expand z around $\frac{2\pi}{\gamma}$: $z((2j-1)\pi/m) = z(2\pi/\gamma) + z'(x_j)\left(\frac{(2j-1)\pi}{m} - \frac{2\pi}{\gamma}\right)$ for some $x_j \in \left[\frac{(2j-1)\pi}{m}, \frac{2\pi}{\gamma}\right]$. The remainder R_m is

$$R_m = z(\tfrac{2\pi}{\gamma})\textstyle\sum_{j=m/\gamma-r+1}^{m/\gamma} e^{i(2j-1)\theta/2} + \sum_{j=m/\gamma-r+1}^{m/\gamma} e^{i(2j-1)\theta/2}\left(\frac{2\pi}{\gamma} - \frac{(2j-1)\pi}{m}\right) z'(x_j). \tag{9}$$

The second sum vanishes in the limit because its absolute value is smaller than $\frac{(2r-1)\pi}{m}\sup|z'(q)|$. The first sum is easily calculated and

$$\lim_{m\to\infty} R_m = z(\tfrac{2\pi}{\gamma}) e^{ir\theta/2}\frac{\sin(r\theta/2)}{\sin(\theta/2)}. \tag{10}$$

The result follows by taking the real and imaginary parts of $\lim(S_m + R_m)$ as given by (8) and (10).
(ii) The result follows from (9) where, again, the second sum goes to zero and the factor $z(\frac{2\pi}{\gamma}) = 0$ removes the r-dependent sum. □

Proposition 3 (Continuous case) *Set $\theta = \frac{2\pi k}{m}$ and denote by* lim *the process of taking the limit $k, m \to \infty$ while keeping θ fixed. The thermodynamical limits of $c^s(k_1,k_2)/c_\uparrow$ (eq. (3)) with $k = k_2 - k_1 > 0$ are*

(i) (supercritical, $\nu < \nu_c$)

$$\lim -\frac{i}{m}\sum_{q\in Q_m} e^{iqk} d(\nu,q) = (1-\tanh 2\nu)(1-\sinh 2\nu)\cosh^2 2\nu,$$

independent of θ;

(ii) (critical, $\nu = \nu_c$)

$$\lim -i\sum_{q\in Q_m} e^{iqk} d(\nu_c,q) = \frac{\sqrt{2}-1}{\sin\theta/2};$$

(iii) (subcritical, $\nu > \nu_c$)

$$\lim -i\sum_{q\in Q_m} e^{iqk} d(\nu,q)$$

goes to a Dirac distribution in the following sense: if $f : \mathbb{T}^1 \to \mathbb{R}$ is a continuous function on the circle, then

$$\lim_{m\to\infty} -i\frac{2\pi}{m}\sum_{k=1}^{m-1} f\left(\frac{2\pi k}{m}\right)\sum_{q\in Q_m} e^{iqk} d(\nu,q) = \gamma f(0)$$

with

$$\gamma = 2\int_0^\pi d(\nu,q)\cot\frac{q}{2}\,dq.$$

We stress that only the properties stated in Lemma 1 are used in the proof and that it is the behavior *(ii)* at $q=0$ that decides between the three regimes.

PROOF: *(critical)* Note that $\lim -i\sum_{q\in Q_m} e^{iqk}d(\nu_c,q) = \lim 2\sum_{q\in Q_m^+} d(\nu_c,q)\sin kq$. By Lemma 1, $d(\nu_c,0^+)=\sqrt{2}-1$ and $d(\nu_c,\pi)=0$ and $d(\nu_c,q)$ is analytic in q for $q\in[0,\pi]$. Therefore the limit follows from Lemma 2 *(ii)*: $\lim -i\sum_{q\in Q_m} e^{iqk}d(\nu_c,q) = \frac{\sqrt{2}-1}{\sin\theta/2}$.

(supercritical) To prove the supercritical case, we first replace the function $d(\nu,q)$ in the limit by $\frac{1}{q}$. Then $-\frac{i}{m}\sum_{q\in Q_m} e^{iqk}\frac{1}{q} = \frac{1}{\pi}\sum_{j=1}^{m/2}\frac{\sin\theta(j-\frac12)}{j-\frac12}$. This sum goes to $\frac{\pi}{2}$ when $m\to\infty$ for any value of $\theta\in(0,2\pi)$. (See [10], App. A, Table II.) Therefore $\lim -\frac{i}{m}\sum_{q\in Q_m} e^{iqk}\frac{1}{q} = \frac12$. Let us write $d(\nu,q)$ as $d(\nu,q)=\frac{\alpha}{q}-\frac{\alpha}{\pi^2}q+g(q)$ where α is the residue of $d(\nu,q)$ at $q=0$: $\alpha = 2(1-\tanh 2\nu)(1-\sinh 2\nu)\cosh^2 2\nu$. Then the new function g is analytic on $[0,\pi]$ with $g(0)=g(\pi)=0$. This function will therefore not contribute to the limit by Lemma 2. (Note that, in the present case, there is even a supplementary factor $\frac{1}{m}$ in the limit.) We thus obtain

$$\lim_{m\to\infty} -\frac{i}{m}\sum_{q\in Q_m} e^{iqk}d(\nu,q) = \frac{\alpha}{2} - \frac{\alpha}{\pi^2}\lim_{m\to\infty} -\frac{i}{m}\sum_{q\in Q_m} qe^{iqk}.$$

Because $|\sum_{j=1}^{m/2}\sin\theta(j-\frac12)| \le 1/|\sin(\theta/2)|$ and $\sum_{j=1}^{m/2} j\sin\theta(j-\frac12)$ grows at most as m times a constant (depending on θ) as $m\to\infty$, the remaining limit on the right-hand side vanishes. The supercritical case follows.

(subcritical) The limit under consideration now is $\lim_{m\to\infty} -\frac{2\pi i}{m}\sum_{k=1}^{m-1} f\left(\frac{2\pi k}{m}\right)\sum_{q\in Q_m} e^{iqk}d(\nu,q)$ for a continuous function f on the circle $\mathbb{T}^1$. The case of a constant function f is simple:

$$\begin{aligned}\lim_{m\to\infty} -\frac{2\pi i}{m}\sum_{k=1}^{m-1} f(0)\sum_{q\in Q_m} e^{iqk}d(\nu,q) &= f(0)\lim_{m\to\infty} -\frac{2\pi i}{m}\sum_{q\in Q_m} d(\nu,q)\sum_{k=1}^{m-1} e^{iqk}\\ &= f(0)\lim_{m\to\infty}\frac{2\pi}{m}\sum_{q\in Q_m} d(\nu,q)\cot\tfrac{q}{2}\end{aligned}$$

and, because $d(\nu,q)$ has a simple zero at $q=0$, the summand is bounded and the limit is $2f(0)\int_0^\pi d(\nu,q)\cot\frac{q}{2}dq$.

We shall now concentrate on the continuous function $g:\mathbb{T}^1\to\mathbb{R}$ given by $g(\theta)=f(\theta)-f(0)$ that vanishes at $\theta=0$:

$$\lim_{m\to\infty} -\frac{2\pi i}{m}\sum_{k=1}^{m-1} g\left(\frac{2\pi k}{m}\right)\sum_{q\in Q_m} e^{iqk}d(\nu,q). \tag{11}$$

First note that the inner sum is an approximation of the Fourier coefficients of $d(\nu,q)$

$$\frac{1}{m}\sum_{q\in Q_m} e^{iqk}d(\nu,q) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{iqk}d(\nu,q)dq + \frac{\text{constant}}{m^2}\frac{\partial^2 d}{\partial q^2}(\nu,q')$$

for some $q' \in [-\pi, \pi]$. With the factor $\frac{1}{m^2}$, the correction terms disappear upon taking the limit. Therefore the limit (11) is $\lim_{m\to\infty} -2\pi i \sum_{k=0}^{m-1} g\left(\frac{2\pi k}{m}\right) d_{-k}$ with $d_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-iqk} d(\nu, q) dq$. Because $d(\nu, q)$ is real-analytic, its Fourier coefficients decrease exponentially, i.e. there exist c_1 and $c_2 > 0$ such that $|d_k| < c_1 e^{-c_2|k|}$, for $k \in \mathbb{Z}$. (See, for example, V.16 of [12].) Let $\epsilon > 0$ and $M = \max_{\theta\in\mathbb{T}^1} |g(\theta)|$. Then there exists $K \in \mathbb{N}$ such that $\left|\sum_{k=K}^{m-1} g\left(\frac{2\pi k}{m}\right) d_{-k}\right| \le c_1 M \frac{e^{-c_2 K}}{1-e^{-c_2}} < \frac{\epsilon}{2}$ for $m > K$. Let $D = \max\{|d_{-1}|, |d_{-2}|, \ldots, |d_{-(K-1)}|\}$. The remaining terms are bounded by $\left|\sum_{k=1}^{K-1} g\left(\frac{2\pi k}{m}\right) d_{-k}\right| < DK \max_{\theta\in[0,\frac{2\pi K}{m}]} |g(\theta)|$. Because g is continuous and $g(0) = 0$, there must be a $N > K$ such that, if $m > N$, then $DK \sup_{\theta\in[0,\frac{2\pi K}{m}]} |g(\theta)| < \frac{\epsilon}{2}$. Therefore the limit (11) vanishes and

$$\lim_{m\to\infty} -\frac{2\pi i}{m} \sum_{k=1}^{m-1} f\left(\frac{2\pi k}{m}\right) \sum_{q\in Q_m} e^{iqk} d(\nu, q) = \gamma f(0) \qquad \text{with} \qquad \gamma = 2\int_0^{\pi} d(\nu, q) \cot \tfrac{q}{2} dq.$$

□

2.3 The discrete and continuous cases for $n < \frac{m}{2}$

We now turn to the general case when the number of spinflips is any number between 0 and m. The calculation for $n = 2$ generalizes trivially to the general case and we give more details for this case. We drop the superindex "s" on $c^s(k_1, k_2, \ldots, k_{2n})$ as it does not play any role here.

To mimick the argument of the previous section, we shall write down the component, in $\xi_q\omega$ (see equation (2)), of the vector v

$$\begin{array}{rcccccccccccccc} & 1 & 2 & 3 & \ldots & k_1-1 & k_1 & k_1+1 & \ldots & k_2-1 & k_2 & k_2+1 & \ldots & m & \\ v = (& - & - & - & \ldots & - & + & + & \ldots & + & - & - & \ldots & - &). \end{array}$$

Because the operators ξ_q's (and η_q's) are made of the operators ρ_k and π_k that flip all spins to the left of the site k and may or may not change the spin k, the only vectors that may contribute to $(\xi_q\omega)_v$ are the seven following (families of) configurations:

	1			k_1			k_2		m
I	$-----$	$\ldots$	$--$	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$
II	$+++--$	$\ldots$	$--$	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$
III	$++++++$	$\ldots$	$++$	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$
IV	$++++++$	$\ldots$	$++$	$---++$	$\ldots$	$++$	$-----$	$\ldots$	$--$
V	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$	$-----$	$\ldots$	$--$
VI	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$	$+++--$	$\ldots$	$--$
VII	$++++++$	$\ldots$	$++$	$-----$	$\ldots$	$--$	$++++++$	$\ldots$	$++$

The configurations I, III, V and VII have 2 spinflips, the others have 4. The action of η_q on these terms in ω is given by $\frac{1}{2} i e^{-i\pi/4} m^{-1/2}$ times

$$
\begin{array}{ll}
\text{I} & -e^{-iq}c(k_1,k_2) \\
\text{II} & \sum_{l=2}^{k_1-1}(e^{-iq(l-1)}-e^{-iql})c(l,k_1,k_2,m+1) \\
\text{III} & (e^{-iq(k_1-1)}+e^{-iqk_1})c(k_2,m+1) \\
\text{IV} & \sum_{l=k_1+1}^{k_2-1}(-e^{-iq(l-1)}+e^{-iql})c(k_1,l,k_2,m+1) \\
\text{V} & (-e^{-iq(k_2-1)}-e^{-iqk_2})c(k_1,m+1) \\
\text{VI} & \sum_{l=k_2+1}^{m}(e^{-iq(l-1)}-e^{-iql})c(k_1,k_2,l,m+1) \\
\text{VII} & e^{-iqm}c(k_1,k_2)
\end{array}
$$

Similar expressions can be obtained for the action of $\eta^\dagger_{-q}$. We shall write the component of v in the equation $\xi_q\omega = (\eta_q\cos\phi_q + \eta^\dagger_{-q}\sin\phi_q)\omega = 0$ in the form

$$\underbrace{\text{II} + \text{IV} + \text{VI}}_{\text{4 spinflips}} = -\Big(\underbrace{(\text{I} + \text{VII}\ ) + \text{III} + \text{V}}_{\text{2 spinflips}}\Big).$$

The left-hand side is

$$ie^{i\pi/4}e^{iq/2}\Big(\underbrace{+\sum_{l=2}^{k_1-1}}_{\text{II}}\ \underbrace{-\sum_{l=k_1+1}^{k_2-1}}_{\text{IV}}\ \underbrace{+\sum_{l=k_2+1}^{m}}_{\text{VI}}\Big)e^{-iql}\sin(\phi_q+q/2)c(\pi(l,k_1,k_2,m+1))$$

where the symbol π appearing in $c(\pi(l,k_1,k_2,m+1))$ is the permutation that orders the integers $l,k_1,k_2,m+1$. One can rewrite compactly this expression by setting $c(k_1,k_2,k_3,k_4) = 0$ whenever two of the arguments coincide and by denoting the parity of the permutation π by $(-1)^{l(\pi)}$:

$$ie^{i\pi/4}e^{iq/2}\sum_{l=2}^{m}(-1)^{l(\pi)}e^{-iql}\sin(\phi_q+q/2)c(\pi(l,k_1,k_2,m+1)). \tag{12}$$

The right-hand side is

$$e^{i\pi/4}e^{iq/2}\cos(\phi_q+q/2)\Big(\underbrace{e^{-iq}c(k_1,k_2)}_{(\text{ I + VII })}\ \underbrace{-e^{-iqk_1}c(k_2,m+1)}_{\text{III}}\ \underbrace{+e^{-iqk_2}c(k_1,m+1)}_{\text{V}}\Big) \tag{13}$$

The discrete inverse Fourier transform gives the desired expression

$$
\begin{aligned}
&(-1)^{l(\pi)}c(\pi(k,k_1,k_2,m+1)) \\
&\qquad = \frac{i}{m}\sum_{q\in Q_m} e^{iqk}d(\nu,q)\left(e^{-iqk_1}c(k_2,m+1) - e^{-iqk_2}c(k_1,m+1) + e^{-iq(m+1)}c(k_1,k_2)\right).
\end{aligned}
$$

The generalization to $2n$ spinflips is immediate. It will be obtained by examining the component of a $(2n-2)$-spinflip configuration in $(\xi_q\omega)$. The contribution of $(2n)$-spinflip

configurations will be of the same form as the left-hand side in (12). (Note that the above calculation depends only on the positions k_1 and k_2 and on the number of stretches of constant signs that are flipped by the operators ρ_k and π_k.) Similarly the $(2n-2)$-spinflip configurations will lead to $(2n-1)$ terms with alternating sign as in (13). We therefore get the following recursive formula.

PROPOSITION 4 (RECURSIVE FORM) *Let the number $2n$ of spinflips be such that $1 \le n \le \frac{m}{2}$ and let $1 \le k_1 < k_2 < \cdots < k_{2n} \le m$ be their positions. Then*

$$c(k_1, k_2, \ldots, k_{2n}) = \frac{i}{m} \sum_{q \in Q_m} \sum_{j=2}^{2n} d(\nu, q) e^{iq(k_1 - k_j)} (-1)^j c(\widehat{k_1}, k_2, \ldots, k_{j-1}, \widehat{k_j}, k_{j+1}, \ldots, k_{2n}) \quad (14)$$

where $c(\widehat{k_1}, k_2, \ldots, k_{j-1}, \widehat{k_j}, k_{j+1}, \ldots, k_{2n}) = c(k_2, k_3, \ldots, k_{j-1}, k_{j+1}, \ldots, k_{2n})$, if $n \ge 2$ and $c_\uparrow$ when $n = 1$.

We restrict the discussion of the thermodynamical limit to the critical regime.

PROPOSITION 5 (CONTINUOUS CASE AT CRITICALITY) *Set $\theta_i = 2\pi k_i/m, 1 \le i \le 2n$ with $n \ge 2$ and denote by* lim *the process of taking the limit $k_1, k_2, \ldots, k_{2n}, m \to \infty$ while keeping the θ_i's fixed. The thermodynamical limit of $c(k_1, k_2, \ldots, k_{2n})$ is*

$$p(\theta_1, \theta_2, \ldots, \theta_{2n}) = \lim \frac{m^n}{c_\uparrow} c(k_1, k_2, \ldots, k_{2n}) = \sum_{j=2}^{2n} \frac{(-1)^j(\sqrt{2}-1)}{\sin(\theta_{j1}/2)} p(\widehat{\theta_1}, \theta_2, \ldots, \widehat{\theta_j}, \theta_{j+1}, \ldots, \theta_{2n})$$

where $\theta_{ij} = \theta_i - \theta_j$ and $p(\widehat{\theta_1}, \theta_2, \ldots, \theta_{j-1}, \widehat{\theta_j}, \theta_{j+1}, \ldots, \theta_{2n}) = p(\theta_2, \theta_3, \ldots, \theta_{j-1}, \theta_{j+1}, \ldots, \theta_{2n})$ if $n \ge 2$ and $= 1$ when $n = 1$.

PROOF: This follows from Proposition 3 for $\nu = \nu_c$ and the elementary fact that the limit of a product is the product of the limits as long as these limits exist. □

As an example we give the continuous case for $n = 2$:

$$p(\theta_1, \theta_2, \theta_3, \theta_4) = (\sqrt{2}-1)^2 \left(\frac{1}{\sin \frac{1}{2}\theta_{12} \sin \frac{1}{2}\theta_{34}} - \frac{1}{\sin \frac{1}{2}\theta_{13} \sin \frac{1}{2}\theta_{24}} + \frac{1}{\sin \frac{1}{2}\theta_{14} \sin \frac{1}{2}\theta_{23}} \right). \quad (15)$$

This particular case was used in [2] to obtain the probability that the interface, separating the constant-spin clusters meeting at θ_1, ends at θ_2.

3 The distribution of the number of spinflips

Is there a "typical" number of spinflips at the boundary of a long cylinder? Or more precisely, what is the probability distribution of the random variable

$$Y_m = \frac{n}{m} = \frac{\#\ \text{spinflips}/2}{\#\ \text{sites at the boundary}} \in [0, \frac{1}{2}]$$

as $m \to \infty$? De Coninck [6] proved that the rescaled variable Y_m is Gaussian in the limit. We use the results of the previous section to recover this and to determine explicitly the mean and variance.

Proposition 6 *The random variable $Y_m = n/m$ on the set of configurations at the extremity of a half-infinite cylinder behaves at criticality as*

$$\lim_{m\to\infty} \mathrm{Pr}_m \left(\frac{Y_m - \mu}{\sigma/\sqrt{m}} < x \right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-x^2/2} dx$$

with $\mu = \frac{1}{2} - \frac{1}{2\pi}(\sqrt{2}+1)$ and $\sigma^2 = \frac{1}{2\pi}(7+5\sqrt{2}) - \frac{3}{8}(3+2\sqrt{2})$.

In particular the above proposition asserts that, at the boundary of a long cylinder covered by a square lattice, there are on average $2m\,\mu \approx 2m \times 0.115766\ldots$ spinflips, that is there is one at almost every 4 sites!

Proposition 5 gives the limit of the discrete probability $\mathrm{P}r_m(k_1 < k_2 < \cdots < k_{2n}|n)$ for the square lattice. Unfortunately the weight included in the limit process (proportional to m^n) rules out comparing relative probabilities of all configurations with a given number of spinflips. One has therefore to go back to the recursive form of Proposition 4 for the probability $c^s(k_1, k_2, \ldots, k_{2n})$ for finite n and m. One may restrict the comparison to configurations whose spin at position 1 is $+$ and again drop the superindex s. We shall use the notation $d(q)$ for $d(\nu_c, q)$. We are interested in computing

$$\lim_{\substack{n,m\to\infty \\ n/m=\kappa \text{ fixed}}} \mathrm{Pr}_m(Y_m = n/m) \tag{16}$$

where $\mathrm{Pr}_m(Y_m = n/m) = \sum_{1\le k_1<k_2<\cdots<k_{2n}\le m} c(k_1, k_2, \ldots, k_{2n})$. The recursive formula (14) can be used to give an explicit expression of $c(k_1, k_2, \ldots, k_{2n})$ as a sum over certain permutations:

$$\mathrm{Pr}_m(Y_m = n/m) = \frac{c_\uparrow}{n!} \sum_{\substack{q_1,q_2,\ldots,q_n\in Q_m^+ \\ \text{distinct } q\text{'s}}} \prod_{1\le j\le n} d(q_j) \cot \tfrac{1}{2} q_j \tag{17}$$

We first prove Proposition 6 using (17).

Proof: We define $f(q) := d(q)\cot(q)$ for short. It is easily checked that the above expression can be rewritten in the form of the probability of n successes for $m/2$ independent Bernoulli trials, each with probability $p_{m,i} := f(q_i)/(1+f(q_i))$ so $1 - p_{m,i} = 1/(1+f(q_i))$. As a result the normalization is $\frac{n!}{c_\uparrow} = \prod_{i=1}^{m/2}(1+f(q_i))$. Let us write $\epsilon_{m,i}$ for a Bernouilli variable with probability $p_{m,i}$. Y_m is then simply $\frac{1}{m}\sum_i^{m/2} \epsilon_{m,i}$. Note that the variables $\epsilon_{m,i}$ form a triangular array. (See, for example, [4].) Moreover they are independent. Therefore the central limit theorem can be applied if the Lindeberg condition is verified. Since the variables $\epsilon_{m,i}$ are uniformly bounded, the condition reduces to verify that the limit of the variance of $\sqrt{m}Y_m$ exists. But we have

$$\sigma^2 := \lim_{m\to\infty} \frac{1}{m} \sum_{i=1}^{m/2} p_{m,i}(1-p_{m,i}) = \frac{1}{2\pi} \int_0^\pi \frac{f(q)}{(1+f(q))^2} dq.$$

In addition, the mean of Y_m converges to

$$\mu := \lim_{m\to\infty} \frac{1}{m} \sum_{i=1}^{m/2} \epsilon_{m,i} = \frac{1}{2\pi} \int_0^\pi \frac{f(q)}{1+f(q)} dq,$$

The integrands in the expression of μ and σ can be put into simple forms:

$$\begin{aligned}
\frac{f(q)}{1+f(q)} &= -\frac{1}{2}(1+\sqrt{2})\left(1-2\sqrt{2}+\cos q+\sqrt{(1-\cos q)(3-\cos q)}\right)\\
\frac{f(q)}{(1+f(q))^2} &= \frac{1}{8\pi(3-2\sqrt{2})}\Big((-2-2\sqrt{2})+(4+2\sqrt{2})\cos q-2\cos^2 q\\
&\qquad\qquad +(2\sqrt{2}-2\cos q)\sqrt{(1-\cos q)(3-\cos q)}\Big).
\end{aligned}$$

Integration can then be done and give $\mu = \frac{1}{2}-\frac{1}{2\pi}(\sqrt{2}+1) \approx 0.115766\ldots$ and $\sigma^2 = \left(\frac{1}{2\pi}(7+5\sqrt{2})-\frac{3}{8}(3+2\sqrt{2})\right) \approx 0.0538198\ldots$. □

We turn now to the proof of (17). Let S_{2n} denote the permutation groups of $2n$ elements. We shall call *pfaffian* a permutation $\pi \in S_{2n}$ of the integers $\{1,2,\ldots,2n\}$ that satisfies

$$\begin{array}{ccccccc}
\pi(1)<\pi(2), & & \pi(3)<\pi(4), & & \ldots, & & \pi(2n-1) < \pi(2n)\\
\pi(1) & < & \pi(3) & < & \ldots & < & \pi(2n-1).
\end{array} \tag{18}$$

(These are the conditions on the indices of terms appearing in the pfaffian of an anti-symmetric $2n\times 2n$ matrix. See, for example, [16, 7] or [11].) The set of all these permutations $\subset S_{2n}$ will be denoted Pf_{2n}. Two well-known facts are useful here. First suppose that $\pi(1)\neq 1$. Then there exists $i>1$ such that $\pi(i)=1$. If i is even, then $\pi(i-1)<\pi(i)$ and one of the pfaffian inequalities is surely false. If i is odd, then it is $\pi(i-2)<\pi(i)$ that is false. Therefore $\pi(1)=1$ for $\pi\in\mathrm{Pf}_{2n}$. Second we obtain the cardinality of Pf_{2n}. We have just seen that $\pi(1)=1$. All values $2\le i\le 2n$ are possible choices for $\pi(2)$. There are $(2n-1)$ of them. By an argument similar to the one leading to $\pi(1)=1$, one shows that $\pi(3)$ must be the smallest integer left in $\{1,2,\ldots,2n\}$ after deletion of $\pi(1)$ and $\pi(2)$. There are then $(2n-3)$ choices for $\pi(4)$. Repeating the argument one gets $|\mathrm{Pf}_{2n}|=(2n-1)!!$ $(<|S_{2n}|=(2n)!)$.

Note that the previous argument for the cardinality of Pf_{2n} follows the process by which the recursive expression (14) constructs the general term of $c(k_1,k_2,\ldots,k_{2n})$. For example, $c(k_1,k_2,k_3,k_4)$ is given by

$$c_\uparrow\left(\frac{i}{m}\right)^2\sum_{q_1,q_2\in Q_m} d(q_1)d(q_2)\left(e^{iq_1(k_1-k_2)}e^{iq_2(k_3-k_4)}-e^{iq_1(k_1-k_3)}e^{iq_2(k_2-k_4)}+e^{iq_1(k_1-k_4)}e^{iq_2(k_2-k_3)}\right).$$

The permutations $(\pi(1),\pi(2),\pi(3),\pi(4))$ appearing here are precisely the three pfaffian permutations of Pf_4. To obtain a similar form for a general n, let us denote the momentum introduced at the j-th use of the recursion formula by q_j and the two indices on the positions k's by $\pi(2j-1)$ and $\pi(2j)$. At the first use the formula (14) forces $\pi(1)$ to be 1 and $\pi(2)$ to be any number between 2 and $2n$. This first step gives rise to the $(2n-1)$ terms $(-1)^i e^{iq_1(k_1-k_i)}$. At the second use, $\pi(3)$ will be the smallest of the remaining integers in $\{1,2,\ldots,2n\}$ and $\pi(4)$ will take any of the $(2n-3)$ remaining values. It is clear then that the indices $\pi(2j-1)$ and $\pi(2j)$ appearing in $\prod_{1\le j\le n} e^{iq_j(k_{\pi(2j-1)}-k_{\pi(2j)})}$ are those obtained by a pfaffian permutation of $\{1,2,\ldots,2n\}$ and that all such permutations occur precisely once.

Because $(i-2)$ is the number of neighbor transpositions necessary to go from $(1, 2, \ldots, 2n)$ to $(1, i, 2, 3, \ldots, i-1, i+1, \ldots, 2n)$, the products of the factors $(-1)^i$ of (14) is simply $(-1)^{l(\pi)}$ where $l(\pi)$ is the parity of π. One can therefore rewrite $c(k_1, k_2, \ldots, k_{2n})$ as follows.

Proposition 5 (Combinatorial form) *Let the number $2n$ of spinflips be such that $1 \leq n \leq \frac{m}{2}$ and let $1 \leq k_1 < k_2 < \cdots < k_{2n} \leq m$ be their positions. Then*

$$c(k_1, k_2, \ldots, k_{2n}) = c_\uparrow \left(\frac{i}{m}\right)^n \sum_{q_1, q_2, \ldots, q_n \in Q_m} \sum_{\pi \in \mathrm{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1 \leq j \leq n} d(q_j) e^{iq_j(k_{\pi(2j-1)} - k_{\pi(2j)})}. \tag{19}$$

The probability $\mathrm{Pr}_m(Y_m = n/m)$ is then

$$\begin{aligned}\mathrm{Pr}_m&(Y_m = n/m) \\ &= c_\uparrow \left(\frac{i}{m}\right)^n \sum_{q_1, q_2, \ldots, q_n \in Q_m} \prod_{1 \leq \ell \leq n} d(q_\ell) \sum_{1 \leq k_1 < k_2 < \cdots < k_{2n} \leq m} \sum_{\pi \in \mathrm{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1 \leq j \leq n} e^{iq_j(k_{\pi(2j-1)} - k_{\pi(2j)})}.\end{aligned} \tag{20}$$

Those familiar with classical works on the Ising model will not be surprised to see a pfaffian sum appearing here. (See, for example, [13].) The continuous limit of (19) can be deduced easily using the result of the previous paragraph. Using Prop. 3 *(ii)*, one finds that the limit of the probability distribution conditionned to the number of spinflips is up to a constant

$$\sum_{\pi \in \mathrm{Pf}_{2n}} \prod_{1 \leq j \leq n} \sin\left(\frac{1}{2}(\theta_{\pi(2j)} - \theta_{\pi(2j-1)})\right). \tag{21}$$

This expression already exists in the literature, though in a slightly different form. Burkhardt and Guim [5] computed the correlation function $\langle \phi_1(z_1, \bar{z}_1) \ldots \phi_a(z_a, \bar{z}_a) \rangle_{\zeta_1, \ldots, \zeta_b}$ of fields ϕ_i, $1 \leq i \leq a$, in the upper-half plane when piecewise constant boundary conditions are applied along the real axis, with spinflips at ζ_j, $1 \leq j \leq b$. If the ϕ_i's are taken to be the identity, one can argue that $\langle \mathbf{1} \rangle_{\zeta_1, \ldots, \zeta_b}$ is nothing but the density probability that spinflips occur at $\zeta_1, \ldots, \zeta_b$. With this identification and after a conformal map of the upper-half plane onto the cylinder (the point at infinity is deleted), their expression (16a) is the above expression (21). Theirs is obtained from conformal field theory, ours from the original definition of the Ising model.

It is interesting to remark that only the outer sum on $q_1, q_2, \ldots, q_n \in Q_m$ contains the information about the temperature, through the function d. The rest of the expression is completely combinatorial in nature and rests only upon the introduction of the anti-commuting (fermionic) operators ξ_q of Section 2 in Onsager's solution. Even though they were introduced for the square lattice, we will see in Section 4 that similar operators exist for the triangular and hexagonal lattices. It is therefore likely that these operators ξ_q may be introduced for a large class of two-dimensional lattices and that their commutation relations are independent of the lattice. The function d, on the other hand, is likely to depend on the lattice. It it therefore natural to introduce the function

$$\widehat{N_n}(q_1, q_2, \ldots, q_n) = \sum_{1 \leq k_1, k_2, \ldots, k_{2n} \leq m} \sum_{\pi \in \mathrm{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1 \leq j \leq n} e^{iq_j(k_{\pi(2j-1)} - k_{\pi(2j)})}.$$

We were not able to find any tractable form for this expression. However note that this expression is to appear within the sum $\sum_{q_j}\prod_\ell d(q_\ell)$ where the dependency on all q's is symmetric. If one decomposes $\widehat{N_n}$ into its S_n-symmetric component, only the fully symmetric one will contribute to the sum over the q's. Moreover, because the function $d(q)$ is an odd function of q, it is sufficient to consider the component in $\widehat{N_n}$ that is odd under the exchange of any of the q's. To be more specific let us introduce the following linear operators. Let $P(q)$ be a polynomial in e^{iq} and e^{-iq}. The linear operator Odd_q acts as $(\mathrm{Odd}_q\, P)(q) = \frac{1}{2}(P(q)-P(-q))$. If $P(q_1, q_2, \dots, q_n)$ is a polynomial in $e^{\pm iq_1}, e^{\pm iq_2}, \dots, e^{\pm iq_n}$, the linear operator $\mathrm{Sym}_{q_1,q_2,\dots,q_n}$ is defined as $(\mathrm{Sym}_{q_1,q_2,\dots,q_n}\, P)(q_1, q_2, \dots, q_n) = \frac{1}{n!}\sum_{\pi\in S_n} P(q_{\pi(1)}, q_{\pi(2)}, \dots, q_{\pi(n)})$ where S_n is the permutation group of n elements. In terms of these, the desired probability is

$$\mathrm{Pr}_m(Y_m = n/m) = c_\uparrow \left(\frac{i}{m}\right)^n \sum_{q_1,q_2,\dots,q_n\in Q_m} N_n(q_1, q_2, \dots, q_n) \prod_{1\le\ell\le n} d(q_\ell) \tag{22}$$

where

$$\begin{aligned} &N_n(q_1, q_2, \dots, q_n) \\ &\quad = \left(\prod_{1\le i\le n} \mathrm{Odd}_{q_i}\right) \mathrm{Sym}_{q_1,q_2,\dots,q_n} \sum_{1\le k_1<k_2<\cdots<k_{2n}\le m} \sum_{\pi\in\mathrm{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1\le j\le n} e^{i(k_{\pi(2j-1)}-k_{\pi(2j)})q_j}. \end{aligned} \tag{23}$$

This function N_n is defined for any positive integer $n \le \frac{m}{2}$. It is a polynomial in the $e^{\pm iq_j}$. It is similar in nature to the kernels of Dirichlet and Fejér arising in elementary Fourier analysis. Here N_n is for a discrete Fourier transform of multivariate functions whose dependency on their variables (momenta) is symmetric and odd. It is tempting to call it the Ising kernel. It turns out that this quantity has a very simple expression. It is shown in the Appendix that $N_n(q_1, q_2, \dots, q_n)$ vanishes whenever there exist $i \ne j$ such that $q_i^2 = q_j^2$ and is otherwise

$$N_n(q_1, q_2, \dots, q_n) = \frac{1}{n!}\left(-\frac{im}{2}\right)^n \prod_{1\le j\le n} \cot \tfrac{1}{2} q_j. \tag{24}$$

With this, the summand in $\mathrm{Pr}_m(Y_m)$ becomes, up to a constant, $\prod_{1\le j\le n} d(q_j)\cot\frac{1}{2}q_j$ when non-zero. This function is symmetric and even in all q's. The sum can be restricted to q's in $Q_m^+ = Q_m \cap \mathbb{R}^+$ by multiplying by 2^n. And because N_n vanishes whenever some of the q's coincide up to sign, the probability corresponds to equation (17).

After long calculations, an agreement with explicit simulations may be sought for reassurance. The Figure 2 was drawn for that purpose. The cases $m = 30, 48, 60, 99, 157, 200$, 397 and 800 are plotted. They are the results of Monte-Carlo simulations except for the two smallest lattices that represent exact calculations. In the computer experiments the length of the cylinder was twice as long as the circumference and the smallest sample (5×10^5) was for the $m = 800$ cylinder. As an example of measurements of σ, this latter case gave $\hat\sigma = 0.05372$. The reader will notice both even and odd m's here even though the proposition was proved for m even only.

The last result of this section is not a consequence of Proposition 6 as such but it does follow from the technique used in its proof.

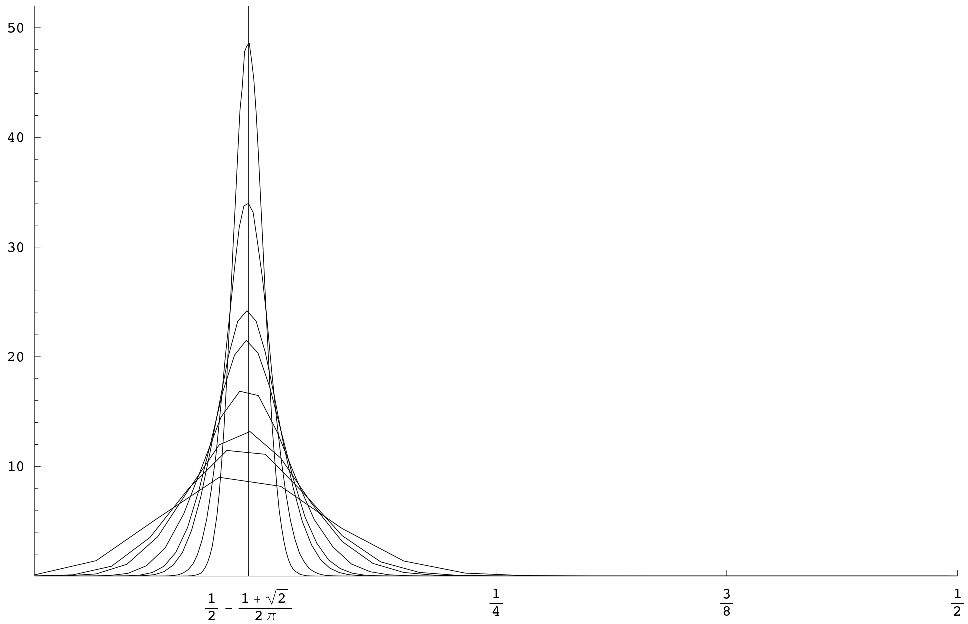

Figure 2: Probability distributions of the variables Y_m for several values of m.

COROLLARY 7 *The probability $c_\uparrow(m)$ of having only spins + at the boundary of a half-infinite cylinder (at the critical temperature) behaves as*

$$c_\uparrow(m) \approx \frac{1}{\sqrt{2}} \left(2(\sqrt{2}-1)e^{2G/\pi}\right)^{-\frac{m}{2}} e^{-\frac{\pi}{24m}} \tag{25}$$

for m large enough. G is Catalan's constant: $G = \sum_{k=0}^{\infty}(-1)^k(2k+1)^{-2}$.

PROOF: The probability $c_\uparrow$ is half the probability of having no spinflip and, by the preceding proof, $c_\uparrow(m) = \frac{1}{2}\Pr(n=0) = (2\prod_{1\le i\le M}(1+f_{M,i}))^{-1}$ with $M = \frac{m}{2}$ and $f_{M,i} = d(q_i)\cot\frac{1}{2}q_i$, $q_i = (2i-1)\pi/m \in Q_m^+$. A direct calculation leads to

$$1 + f(q) = \frac{1}{\sin\frac{q}{2}} \frac{2\sqrt{2} - 1 - \cos q + \sqrt{(1-\cos q)(3-\cos q)}}{2\sqrt{1-\cos q} + \sqrt{2}\sqrt{3-\cos q}}.$$

Using standard tables (see for example paragraph 6.1.2 of [17]), one finds $\prod_{j=1}^{\frac{m}{2}} \sin\frac{q_j}{2} = \frac{1}{2^{(m-1)/2}}$. Therefore

$$\begin{aligned}\prod_{1\le i\le M}(1+f_{M,i}) &= \exp\sum_{1\le i\le M}\log(\sin q_i/2 + d(q_i)\cos q_i/2) - \log(\sin(q_i/2)) \\ &= 2^{(m-1)/2}\exp\sum_{q\in Q_m^+}\log h(q)\end{aligned}$$

where

$$h(q) = \frac{2\sqrt{2} - 1 + \cos q + \sqrt{(1+\cos q)(3+\cos q)}}{2\sqrt{1+\cos q} + \sqrt{2}\sqrt{3+\cos q}}.$$

This function h is the remaining factor in $(1+f)$ evaluated at $\pi - q$. Note that the set Q_m^+ is stable under the operation $q \to \pi - q$. Moreover h has the following useful properties: it is analytic on $(-\pi, \pi)$, even and takes the value 1 at $q = 0$. One can write $\log h(q) = \sum_{i\geq 2,\text{even}} a_i q^i$ and therefore $\sum_{q\in Q_m^+} \log h(q) = \sum_{i\geq 2,\text{even}} a_i \sum_{j=1}^{m/2} q_j^i$. The leading terms (in m) in the inner sum are $\sum_{j=1}^{m/2} q_j^i = \pi^i \left(\frac{m}{2(i+1)} - \frac{1}{12}\frac{i}{m} + \mathcal{O}\left(\frac{1}{m^2}\right)\right)$. The first term can be resummed as follows

$$\sum_{i\geq 2,\text{even}} a_i \frac{\pi^i m}{2(i+1)} = \frac{m}{2\pi} \sum_{i\geq 2,\text{even}} \int_0^\pi a_i x^i dx = \frac{m}{2\pi} \int_0^\pi \log h(q) dq$$

and the second as

$$-\frac{1}{12} \sum_{i\geq 2,\text{even}} a_i \frac{\pi^i i}{m} = -\frac{\pi}{12m} \frac{d}{dq} \log h(q)\bigg|_{q=\pi^-} = \frac{\pi}{24m}.$$

The integral appearing in the first term is again somewhat difficult. Rewriting the integrand as follows and using *Mathematica*, we were able to obtain

$$\int_0^\pi \log h(q) dq = \int_0^\pi \log\left((1 - \frac{1}{\sqrt{2}})(\sqrt{1-\cos q} + \sqrt{3-\cos q})\right) dq = \pi \log(\sqrt{2}-1) + 2G$$

where G is Catalan's constant. Gathering the various terms, we get (25). □

4 Behavior at the boundary for the triangular and hexagonal lattices

In this section we extend the techniques used for the square lattice to compute the quantity $c^s(k_1, k_2)$ for the hexagonal and the triangular cases. These lattices are characterized by a connectivity of 6 and 3 respectively except at the boundary, where more than one choices can be made. Our choice is drawn in figure 3. The square-shaped representation will be helpful for the computations of the transfer matrix that follows.

The main result of the section asserts that the thermodynamic limit of $c^s(k_1, k_2)$ at critical temperature behaves as in the square lattice case. This yields some evidence of the universality of the critical behavior at the boundary.

PROPOSITION 8 *Let m be even, k be such that $1 \leq k \leq 2m$ and set $\theta = \frac{2\pi k}{2m}$. Let p, n and r as in Lemma 2 with $\gamma = 4$. Denote by* lim *the process of taking the limit $k, m \to \infty$ while keeping both θ and r fixed. Then at criticality for $k = k_2 - k_1$*

$$\lim \frac{c^s(k_1, k_2)}{c_\uparrow} = \frac{C_{\text{lattice}}}{\sin \theta/2}$$

where C_{lattice} is either $C_{\text{tri}} = 2(2-\sqrt{3})$ or $C_{\text{hex}} = 4/3$ if k is even and $2(\sqrt{3}-1)/3$ if k is odd.

Even though we focused on the case of two spinflips, it is possible to generalize inductively our result to $c^s(k_1, ..., k_n)$ in the same way as in Section 2. The result would be similar to the square lattice with the appropriate constant C_{lattice}.

The proposition implies that, for the hexagonal lattice, various limits can be obtained for the same θ. To understand this, one should look at Figure 3. For the triangular lattice, a spinflip on an even site is actually equivalent (up to a reflection) to a spinflip on an odd site. This is not true for the hexagonal lattice. The case of a spinflip on an odd site is different from a spinflip on an even site: in the latter the sites are not nearest-neighbors whereas in the first, they are. This asymmetry persists in the continuum limit. A parallel with quantum field theory is useful. It is impossible physically to measure this probability precisely for a given θ. A measurement that *is* possible is to obtain the probability that the two spinflips occur within a distance $\theta \in [\theta_{\min}, \theta_{\max}]$. To calculate this probability (or this "smeared correlation function") from the above result, one would have to use the average of $C_{\text{hex}}^{\text{even}}$ and $C_{\text{hex}}^{\text{odd}}$ as the sites with k even and those with k odd have the same density. (Of course this above limiting distribution is not normalizable and a cut-off becomes necessary.)

We start by reviewing the diagonalization of the transfer matrix in Section 4.1 following the work of Houtappel [14]. Then we construct in Section 4.2 an equation similar to (2) for the eigenvector with the largest eigenvalue. We get, in a similar way as in Section 2, an expression for $c^s(k_1, k_2)$ which involves functions that play the same role as $d(\nu, q)$ in the square case. These functions are investigated only at critical temperature. As before the critical behavior is related to the jump of these functions at $q = 0$.

4.1 Transfer matrix for the triangular and hexagonal lattices

The element of the transfer matrices for our particular choice of lattices and boundaries for a transfer from row σ to row σ' with $2m$ sites (m even), i.e. the difference of Gibbs weights between these two rows, is

$$T_{\text{tri}}(\sigma', \sigma) = \exp\left(\nu\left\{\sum_{j=1}^{2m} \sigma_j \sigma'_j + \sum_{j=1}^{2m} \sigma'_j \sigma'_{j+1} + \sum_{j=1}^{m} (\sigma'_{2j-1} + \sigma'_{2j+1})\sigma_{2j}\right\}\right)$$

$$T_{\text{hex}}(\sigma', \sigma) = \sum_{\sigma^I} \exp\left(\nu\left\{\sum_{j=1}^{2m} (\sigma_j + \sigma'_j)\sigma^I_j + \sum_{j=1}^{m} (\sigma'_{2j-1}\sigma'_{2j} + \sigma^I_{2j}\sigma^I_{2j+1})\right\}\right)$$

where $\sigma_{2m+1} \equiv \sigma_1$ and the sum over σ^I is the sum over all possible configurations of the intermediate row. It is convenient to write the previous expressions in terms of matrices that contain interactions along columns only or along rows only to follow thereafter the calculation for the square lattice. We explain here the triangular case. The hexagonal case is done exactly the same way and only major steps are given.

We decompose the transfer matrix from σ to σ' into the product of several transfer matrices. Figure 4 depicts this process. Dotted bonds represent the identification of two sites (in other words a weight of 1 for the initial state and of 0 for the other state). Plain lines are the usual ferromagnetic bonds. With this particular choice of decomposition interactions along rows and along columns lie in different matrices. One gets the following representation

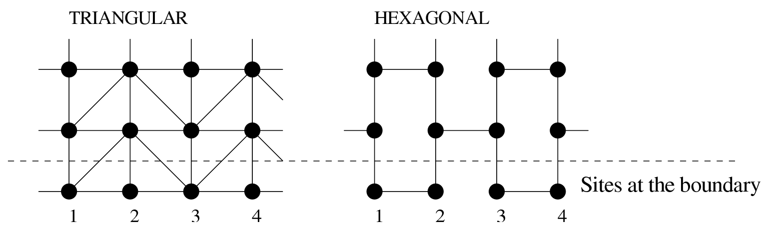

Figure 3: Triangular and hexagonal lattices with our particular choice of boundaries.

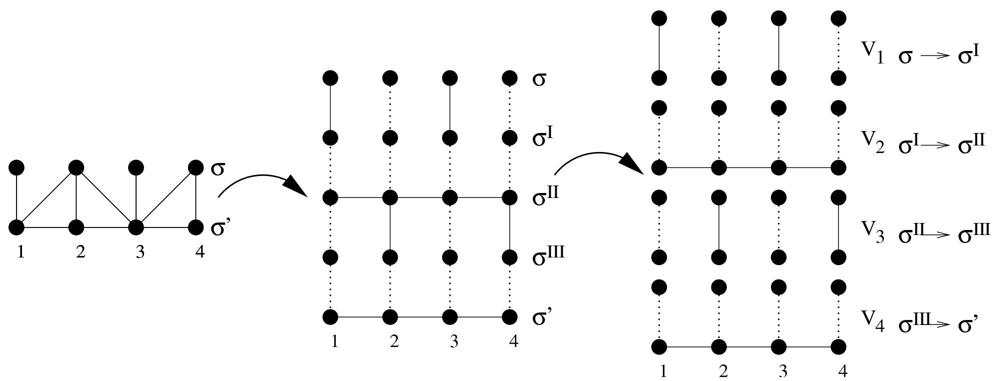

Figure 4: Decomposition of the transfer matrix into V_1, V_2, V_3, V_4 for the triangular case.

of the transfer matrix by summing over all possible intermediate configurations

$$T_{\rm tri}(\sigma',\sigma) = \sum_{\sigma^I,\sigma^{II},\sigma^{III}} V_4(\sigma',\sigma^{III})V_3(\sigma^{III},\sigma^{II})V_2(\sigma^{II},\sigma^I)V_1(\sigma^I,\sigma) \tag{26}$$

where the V_i's are defined as follows

$$\begin{aligned} V_1(\sigma',\sigma) &= \exp\left(\nu\sum_{j\ \rm odd}\sigma_j\sigma'_j\right)\prod_{j\ \rm even}\delta_{\sigma_j,\sigma'_j} \quad V_3(\sigma',\sigma) = \exp\left(\nu\sum_{j\ \rm even}\sigma_j\sigma'_j\right)\prod_{j\ \rm odd}\delta_{\sigma_j,\sigma'_j} \\ V_2(\sigma',\sigma) &= V_4(\sigma',\sigma) = \exp\left(\nu\sum_j\sigma'_j\sigma'_{j+1}\right)\prod_j\delta_{\sigma_j,\sigma'_j}. \end{aligned} \tag{27}$$

Second we rewrite these matrices in terms of the operators τ_k^i, $k = 1,...,2m$ and $i = 1,2,3$, and of the operators π_k, ρ_k and P (all defined in Section 2 and in [18])

$$\begin{aligned} V_1 &= (2\sinh 2\nu)^{m/2}\exp\left(i\nu^*\sum_{j\ \rm odd}\pi_j\rho_j\right) \quad V_3 = (2\sinh 2\nu)^{m/2}\exp\left(i\nu^*\sum_{j\ \rm even}\pi_j\rho_j\right) \\ V_2 &= V_4 = \exp(i\nu\pi_1\rho_{2m}P)\exp\left(-i\nu\sum_{j=1}^{2m-1}\pi_{j+1}\rho_j\right) \end{aligned} \tag{28}$$

where $\sinh\nu\sinh\nu^* = 1$. As in the square case, the parity operator P must commute with each V_i because the Gibbs weights are invariant under $\sigma \to -\sigma$. It is therefore possible to diagonalize simultaneously T and P. Hence we write $T = \frac{1}{2}(1+P)T^+ + \frac{1}{2}(1-P)T^-$ where $T^\pm$ acts in a non-trivial way on the even/odd subspace and has eigenvalue zero for odd/even eigenvectors. Taking this into account in the previous expression of V_2 and replacing π_k and ρ_k by their expression in terms of a_k, we get

$$V_1 = (2\sinh 2\nu)^{m/2}\exp\left(-2\nu^*\sum_{j \text{ odd}} a_j^\dagger a_j - \frac{1}{2}\right) \quad V_3 = (2\sinh 2\nu)^{m/2}\exp\left(-2\nu^*\sum_{j \text{ even}} a_j^\dagger a_j - \frac{1}{2}\right)$$
$$V_2^\pm = V_4^\pm = \exp\left(\nu\sum_j (a_{j+1}^\dagger - a_{j+1})(a_j^\dagger + a_j)\right) \tag{29}$$

with $T_{\text{tri}}^+ = V_4^+ V_3 V_2^+ V_1$ and similarly for T_{tri}^-. The condition of parity imposes $a_{2m+1} = \mp a_1$ for $V^\pm$.

We claim that the eigenvector ω with highest eigenvalue lies in the even subspace. Indeed the operator P flips a configuration σ into $-\sigma$ and it acts as $-I$ in the odd sector. If ω lies in the odd sector, then $P\omega = -\omega$ and its coefficients in the basis of configurations must satisfy: $c_{\sigma_1\sigma_2\ldots\sigma_{2m}} = -c_{-\sigma_1-\sigma_2\cdots-\sigma_{2m}}$. It follows that some coefficients are negative or they are all zero, contradicting Frobenius theorem. We shall thus be interested in diagonalizing T^+.

The particular form of V_i for $i = 2, 4$ leads us to define two Fourier transforms:

$$a_k = \begin{cases} \frac{e^{i\pi/4}}{\sqrt{m}}\sum_{q\in Q_m} e^{ikq}\eta_q, & \text{for } k \text{ odd} \\ \frac{e^{i\pi/4}}{\sqrt{m}}\sum_{q\in Q_m} e^{ikq}\delta_q, & \text{for } k \text{ even} \end{cases}$$
$$\text{where} \quad Q_m = \left\{\frac{(2l-1)\pi}{2m} : -m/2+1 \le l \le m/2\right\}. \tag{30}$$

Again, m is assumed even. The particular definition of Q_m allows us to invert the previous relations to get

$$\eta_q = \frac{e^{-i\pi/4}}{\sqrt{m}}\sum_{k \text{ odd}} e^{-iqk}a_k, \qquad \delta_q = \frac{e^{-i\pi/4}}{\sqrt{m}}\sum_{k \text{ even}} e^{-iqk}a_k. \tag{31}$$

The anti-commutation relations of the a_k induce relations for the Fourier transforms

$$\begin{aligned} \{\eta_q, \eta_{q'}\} = \{\delta_q, \delta_{q'}\} = 0, &\quad \{\eta_q, \delta_{q'}\} = \{\eta_q, \delta_{q'}^\dagger\} = 0, \\ \{\eta_q, \eta_q^\dagger\} = \{\delta_q, \delta_q^\dagger\} = 1, &\quad \{\eta_q, \eta_{q'}^\dagger\} = \{\delta_q, \delta_{q'}^\dagger\} = 0 \quad \text{if } q \neq q'. \end{aligned} \tag{32}$$

These relations decouple the various sectors of momentum q, $-\pi/2 < q < \pi/2$. As we shall now see the V's mix the sector of a given momentum q with that of momentum $-q$, but with no other. Therefore it is possible to express T in terms of a tensor product of operators acting on specific sectors of momenta q and $-q$. A direct substitution of (30) in (29) gives the precise form of these operators. We get $T_{\text{tri}}^+ = (2\sinh 2\nu)^{m/2}\prod_{0<q<\pi/2} V_q$ for

$V_q = V^+_{4,q} V_{3,q} V^+_{2,q} V_{1,q}$ where

$$
\begin{aligned}
V_{1,q} &= \exp\left(-2\nu^*\left(\eta^\dagger_q\eta_q + \eta^\dagger_{-q}\eta_{-q} - 1\right)\right) \quad V_{3,q} = \exp\left(-2\nu^*\left(\delta^\dagger_q\delta_q + \delta^\dagger_{-q}\delta_{-q} - 1\right)\right)\\
V^+_{2,q} = V^+_{4,q} &= \exp\Big(\nu e^{-iq}\Big(-i(\eta^\dagger_q\delta^\dagger_{-q} + \eta_{-q}\delta_q + \delta^\dagger_q\eta^\dagger_{-q} + \delta_{-q}\eta_q)\\
&\qquad + \ (\delta^\dagger_{-q}\eta_{-q} + \eta^\dagger_q\delta_q + \delta^\dagger_q\eta_q + \eta^\dagger_{-q}\delta_{-q})\Big) + \star\Big)
\end{aligned}
\tag{33}
$$

where $\star$ holds for a term identical to the preceding one but with $q \to -q$. A similar calculation of the transfer matrix for the hexagonal case yields

$$
\begin{aligned}
W_{1,q} = W_{3,q} &= \exp\left(-2\nu^*\left((\eta^\dagger_q\eta_q + \delta^\dagger_q\delta_q - 1) + \star\right)\right)\\
W^+_{2,q} &= \exp\left(\nu e^{-iq}\left(-i(\eta^\dagger_q\delta^\dagger_{-q} + \eta_{-q}\delta_q) + (\eta^\dagger_q\delta_q + \delta^\dagger_{-q}\eta_{-q})\right) + \star\right)\\
W_{4,q} &= \exp\left(\nu e^{-iq}\left(-i(\delta^\dagger_q\eta^\dagger_{-q} + \delta_{-q}\eta_q) + (\delta^\dagger_q\eta_q + \eta^\dagger_{-q}\delta_{-q})\right) + \star\right)
\end{aligned}
\tag{34}
$$

for $T^+_{\text{hex}} = (2\sinh 2\nu)^m \prod_{0<q<\pi/2} W_q$ for $W_q = W_{4,q} W_{3,q} W^+_{2,q} W_{1,q}$.

Recall that each V_q and W_q appearing in the tensor product are operators acting on a space labeled by a pair $(q, -q)$ with $q \in Q_m$. Each space (there are $m/2$ in total) is of dimension 2^4. A basis for a given space labeled by q is constructed by applying the fermionic operators $\eta_{\pm q}$, $\delta_{\pm q}$ and their conjugates on the vacuum denoted $|0\rangle$. (It should be stressed that $|0\rangle$ *is not* an eigenvector of V_q. See [22].) One can then recognize five subspaces of a space q that are invariant under the action of V_q and W_q. They are spanned by:

$$
\begin{aligned}
&\{\delta^\dagger_q\eta^\dagger_q|0\rangle\}\\
&\{\eta^\dagger_q|0\rangle, \delta^\dagger_q|0\rangle, \delta^\dagger_{-q}\delta^\dagger_q\eta^\dagger_q|0\rangle, \delta^\dagger_q\eta^\dagger_{-q}\eta^\dagger_q|0\rangle\},\\
&\{|0\rangle, \delta^\dagger_{-q}\eta^\dagger_q|0\rangle, \delta^\dagger_q\eta^\dagger_{-q}|0\rangle, \delta^\dagger_{-q}\delta^\dagger_q|0\rangle, \eta^\dagger_{-q}\eta^\dagger_q|0\rangle, \delta^\dagger_{-q}\delta^\dagger_q\eta^\dagger_{-q}\eta^\dagger_q|0\rangle\},\\
&\{\eta^\dagger_{-q}|0\rangle, \delta^\dagger_{-q}|0\rangle, \delta^\dagger_{-q}\delta^\dagger_q\eta^\dagger_{-q}|0\rangle, \delta^\dagger_{-q}\eta^\dagger_{-q}\eta^\dagger_q|0\rangle\},\\
&\{\delta^\dagger_{-q}\eta^\dagger_{-q}|0\rangle\}.
\end{aligned}
\tag{35}
$$

We will refer to these subspaces respectively as subspaces of momentum $2q$, q, 0, $-q$ and $-2q$. Because the highest eigenvalue of the transfer matrix T is not degenerate, none of the highest eigenvalue of the V_q's can be either. Hence, because the actions of V_q on the subspaces of momenta q and $-q$ are identical (similarly for $2q$ and $-2q$), ω must lie in the subspace of momentum 0. To get ω, it thus remains to diagonalize the block acting on the space of momentum 0, which is of dimension 6. This can be done by writing the representation of V_q in this subspace in the basis (35). Symbolic manipulation programs can be used to take exponentials and to perform the diagonalization. We will not write these expressions here but they will be used in the next section to compute $c^s(k_1, k_2)$.

4.2 Computation of $c^s(k_1, k_2)$

The first step in computing $c^s(k_1, k_2)$ is to construct two operators that annihilate ω, instead of one for the square lattice. It then remains to apply them to ω in the basis of the spinflips

to get $c^s(k_1,k_2)$. We will need three important facts. The results apply to both the hexagonal and triangular cases. V_q stands here for either V_q or W_q.

LEMMA 9 *For all $q>0$ in Q_m, the operator V_q satisfies the relation $\phi_q^T V_q^T \phi_q V_q = 1$ where $\phi_q = \left(\delta_q^\dagger + \delta_q\right)\left(\delta_{-q}^\dagger + \delta_{-q}\right)\left(\eta_q^\dagger + \eta_q\right)\left(\eta_{-q}^\dagger + \eta_{-q}\right)$ and "^{T}" denotes the transposed operator.*

PROOF: By definition of δ_q and η_q in terms of Pauli matrices, one gets $\phi_q^T = \phi_q$ and $\phi_q^2 = 1$. Hence it suffices to show that $\phi_q^T V_{i,q}^T \phi_q V_{i,q} = 1$, $i = 1,2,3,4$. This is directly verified by expressing every operator in terms of δ_q and η_q and by using their anti-commutation relations (32). □

PROPOSITION 10 *Let ω_1 and ω_2 be two eigenvectors of V_q with eigenvalues λ_1 and λ_2 respectively. Then either $\lambda_1 = 1/\lambda_2$ or $(\omega_1,\omega_2)_{\phi_q} = 0$, where $(\ \cdot\ ,\ \cdot\ )_{\phi_q}$ is the bilinear form induced by ϕ_q: $(u,v)_{\phi_q} \equiv u^T\phi_q v$.*

PROOF: By direct calculations, using Lemma 9. □

COROLLARY 11 *If v_q is an eigenvector of V_q with eigenvalue $\lambda \neq 1$, then $(v_q,v_q)_{\phi_q} = 0$.*

We note that the subspace of momentum 0 is an invariant subspace of ϕ_q so that the corollary holds on this subspace. If ω_q denotes the component of ω in the subspace q of momentum 0, we must have by the corollary that $(\omega_q,\omega_q)_{\phi_q} = 0$, since the action of V_q and W_q on the subspace is different than the identity. In the basis of (35), this becomes for $\omega_q = (v_1,v_2,v_3,v_4,v_5,v_6)$

$$v_1v_6 - v_2v_3 - v_4v_5 = 0. \tag{36}$$

We stress that all the above statements hold at any temperature.

The desired operators are now constructed. By analogy with the square case we choose the form

$$\xi_q = a\eta_q + b\delta_q + c\eta_{-q}^\dagger + d\delta_{-q}^\dagger. \tag{37}$$

where a, b, c, d may depend on q. We argued previously that ω belongs to the subspace of momentum 0. Hence, from the definition of ξ_q, $\xi_q\omega_q$ must lie in the subspace of momentum $-q$. The equation $\xi_q\omega_q = 0$ written in the basis (35) becomes in this 4-dimensional subspace

$$\begin{pmatrix} v_5 & -v_3 & -v_1 & 0 \\ -v_2 & -v_4 & 0 & v_1 \\ -v_6 & 0 & v_4 & v_3 \\ 0 & v_6 & v_2 & -v_5 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = 0.$$

If we assume that the components v_i of ω are non-zero, then the 4×4 matrix above can be shown to be of rank 2 by (36). It is easily checked that the kernel is spanned by $(-v_2,v_5,0,v_6)$ and $(v_4,-v_2,v_6,0)$. These vectors yield the two desired operators that we now refer to as ξ_q and ξ_q' respectively.

The coefficient $c^s(k_1,k_2)$ can now be calculated as in section 2. We first write ω in the basis of the spinflips: $\omega = c_\uparrow\sigma_\uparrow + c_\downarrow\sigma_\downarrow + \sum_{l=1}^n \sum_{1\le k_1<\ldots<k_{2l}\le 2m} c^\pm(k_1,\ldots,k_{2l})(\pm;k_1,\ldots,k_{2l})$. We compute the action of ξ_q and ξ_q', $0<q<\pi/2$, on ω in the space of momentum 0 taking

ξ_q and ξ'_q in the form (37). We recall that the action of these operators is well understood in the basis of spinflips if one writes ξ_q and ξ'_q in terms of operator π_k and ρ_k that change the sign of the spins from the site 1 to $k-1$ and from 1 to k respectively. The result of the action must be 0. We calculate $c^{\pm}(1,k)$ and $c^{\pm}(k_1,k_2)$ follows by translational invariance. The projections of $\xi_q\omega$ and $\xi'_q\omega$ on $\sigma_\uparrow$ yield two equations:

$$\begin{aligned} c_\uparrow\left(-v_3e^{-iq}-v_5-iv_6\right) &= \sum_{k \text{ even}} c^-(1,k)e^{-iqk}\left(-v_3e^{iq}+v_5-iv_6\right)\\ &+\sum_{k \text{ odd}} c^-(1,k)e^{-iqk}\left(v_3-v_5e^{iq}-iv_6e^{iq}\right)\\ c_\uparrow\left(-v_4e^{-iq}+v_2+iv_6e^{-iq}\right) &= \sum_{k \text{ even}} c^-(1,k)e^{-iqk}\left(-v_4e^{iq}-v_2-iv_6e^{-iq}\right)\\ &+\sum_{k \text{ odd}} c^-(1,k)e^{-iqk}\left(v_4+v_2e^{iq}-iv_6\right). \end{aligned} \tag{38}$$

These two equations can be solved for $\sum_{k \text{ odd}} c^-(1,k)$ and $\sum_{k \text{ even}} c^-(1,k)$. The inverse Fourier transform on q yields $c^-(1,k)$. By translational invariance, we get for any k_1, k_2:

$$c^s(k_1,k_2)=\begin{cases}\frac{-i}{2m}\sum_{q\in Q_m} e^{iq(k_2-k_1)}d_{\text{even}}(\nu,q), & \text{if } k_2-k_1+1 \text{ is even},\\ \frac{-i}{2m}\sum_{q\in Q_m} e^{iq(k_2-k_1)}d_{\text{odd}}(\nu,q), & \text{if } k_2-k_1+1 \text{ is odd},\end{cases} \tag{39}$$

where

$$\begin{aligned} d_{\text{even}}(\nu,q) &= \frac{-2(v_1+v_6)+2i(v_5-v_4)}{\sin q(v_6-v_1)-\cos q(v_4+v_5)+(v_3-v_2)},\\ d_{\text{odd}}(\nu,q) &= \frac{2\cos q(1-v_1)+2\sin q(v_4+v_5)+2i(v_2+v_3)}{\sin q(v_6-v_1)-\cos q(v_4+v_5)+(v_3-v_2)}. \end{aligned}$$

The components $v_1,\dots,v_6$ of ω_q are obtained following Section 4.1. The expressions for a generic temperature ν are rather heavy. We write down the result for $\nu=\nu_c$. The use of symbolic manipulation programs was essential to obtain the expressions in these relatively simple forms.

Triangular Lattice

$$\begin{aligned} d^{\text{tri}}_{\text{even}}(\nu_c,q) &= \begin{cases}\frac{2\left(-3-\sin q+2\left(\cos\frac{q}{2}+\sin\frac{q}{2}\right)\sqrt{3+\sin q}\right)+2i\left(2\cos q-\left(\cos\frac{q}{2}-\sin\frac{q}{2}\right)\sqrt{3+\sin q}\right)}{\sqrt{3}(1+3\sin q)}, & \text{if } 0\le q\le\frac{\pi}{2};\\ -\text{Re}\left[d^{\text{tri}}_{\text{even}}(\nu_c,-q)\right]+i\ \text{Im}\left[d^{\text{tri}}_{\text{even}}(\nu_c,-q)\right], & \text{if } -\frac{\pi}{2}\le q<0;\end{cases}\\ d^{\text{tri}}_{\text{odd}}(\nu_c,q) &= \begin{cases}\frac{4\left(\cos\frac{q}{2}-\sin\frac{q}{2}\right)\left(\cos\frac{q}{2}+\sin\frac{q}{2}-\frac{1}{2}\sqrt{3+\sin q}\right)}{1+3\sin q}, & \text{if } 0\le q\le\frac{\pi}{2};\\ -d^{\text{tri}}_{\text{odd}}(\nu_c,-q), & \text{if } -\frac{\pi}{2}\le q<0.\end{cases} \end{aligned} \tag{40}$$

Hexagonal Lattice

$$\begin{aligned} d^{\text{hex}}_{\text{even}}(\nu_c,q) &= \begin{cases}-\frac{2\left(\sqrt{3}-1\right)\left(3+\sin q-\sqrt{3}\left(\cos\frac{q}{2}+\sin\frac{q}{2}\right)\sqrt{3+\sin q}\right)}{\sin q(3+\sin q)}, & \text{if } 0\le q\le\frac{\pi}{2};\\ -d^{\text{hex}}_{\text{even}}(\nu_c,-q), & \text{if } -\frac{\pi}{2}\le q<0;\end{cases}\\ d^{\text{hex}}_{\text{odd}}(\nu_c,q) &= \begin{cases}\frac{\left(\cos\frac{q}{2}-\sin\frac{q}{2}\right)\left(-2\sqrt{3}\sqrt{3+\sin q}+2\left(\cos\frac{q}{2}+\sin\frac{q}{2}\right)(3+\sin q)\right)}{\sin q(3+\sin q)}, & \text{if } 0\le q\le\frac{\pi}{2};\\ -d^{\text{hex}}_{\text{odd}}(\nu_c,-q), & \text{if } -\frac{\pi}{2}\le q<0.\end{cases} \end{aligned} \tag{41}$$

We gather in a lemma the properties of the above functions that are relevant for the limit $m \to \infty$. Its proof is similar to that of Lemma 1. The continuum limit of $2mc^s(k_1, k_2)/c_\uparrow$ in Proposition 8 follows directly from Lemmas 2 and 12, with $r\theta = 2\pi k/\gamma = \pi k/2$.

Lemma 12 *The four functions $d^{\text{tri}}_{\text{odd}}$, $d^{\text{tri}}_{\text{even}}$, $d^{\text{hex}}_{\text{odd}}$, $d^{\text{hex}}_{\text{even}}$ on $[-\frac{\pi}{2}, \frac{\pi}{2}]$ have the following properties:*
(i) *their restriction to $[0, \frac{\pi}{2}]$ satisfy the requirements put on z in Lemma 2;*
(ii) *their parity and some of their relevant values are as follows.*

	values in		parity	$(\nu_c, 0^+)$	$(\nu_c, \frac{\pi}{2})$
$d^{\text{tri}}_{\text{odd}}$	$\mathbb{R}$		odd	$2(2-\sqrt{3})$	0
$d^{\text{tri}}_{\text{even}}$	$\mathbb{C}$	Re $d^{\text{tri}}_{\text{even}}$	odd	$2(2-\sqrt{3})$	
		Im $d^{\text{tri}}_{\text{even}}$	even	$2(2-\sqrt{3})$	0
$d^{\text{hex}}_{\text{odd}}$	$\mathbb{R}$		odd	$\frac{4}{3}$	0
$d^{\text{hex}}_{\text{even}}$	$\mathbb{R}$		odd	$\frac{2}{3}(\sqrt{3}-1)$	

We were not able to bring the expressions for a generic temperature ν into a form suitable for publication. Like the function d of the square lattice (eq. (4)), they seem to have an interval of discontinuity in the (ν, q)-plane extending from $(0,0)$ to $(\nu_c, 0)$. This is shown on Figure 5 where the real part of $d^{\text{tri}}_{\text{even}}$ has been plotted. Because of the singularity along the interval with $q = 0$ and $\nu \in (0, \nu_c]$, we have to limit the range (vertical axis) to the interval $[-0.8, 0.8]$. The cut on the surface imposed by this limitation has been marked by a darker curve. The restrictions of Re $d^{\text{tri}}_{\text{even}}(\nu, q)$ to three values of ν have been also highlighted. These three values are $\nu_c + \frac{1}{40} = 0.299653\ldots$ in the subcritical phase, the critical value $\nu_c = 0.274653\ldots$ and $\nu_c - \frac{1}{40} = 0.249653\ldots$ in the supercritical phase. The subcritical curve is obviously smooth. Lemma 12 has established that the cricital curve is real-analytic except at $q = 0$ where there is a jump: Re $d^{\text{tri}}_{\text{even}}(\nu_c, 0^+) = -$Re $d^{\text{tri}}_{\text{even}}(\nu_c, 0^-) = 2(2-\sqrt{3})$. The supercritical curve seems to have a pole at $q = 0$.

Appendix: A combinatorial lemma

The purpose of this appendix is to show the following lemma.

Lemma 13 (Ising kernel) *Let m be a positive even integer and n a positive integer such that $2n \le m$. The polynomial $N_n(q_1, q_2, \ldots, q_n)$ in $e^{\pm iq_1}, e^{\pm iq_2}, \ldots, e^{\pm iq_n}$ defined by*

$$\left(\prod_{1\le i\le n} \text{Odd}_{q_i}\right) \text{Sym}_{q_1,q_2,\ldots,q_n} \sum_{1\le k_1<k_2<\cdots<k_{2n}\le m} \sum_{\pi\in\text{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1\le j\le n} e^{i(k_{\pi(2j-1)}-k_{\pi(2j)})q_j} \tag{42}$$

is

$$= \begin{cases} 0, & \text{if there exists } i \ne j \text{ such that } q_i^2 = q_j^2, \\ \dfrac{1}{n!}\left(-\dfrac{im}{2}\right)^n \displaystyle\prod_{1\le j\le n} \cot \tfrac{1}{2} q_j, & \text{otherwise,} \end{cases}$$

when the values of the q's are restricted to the set $Q_m = \{(2j-1)\pi/m, -\frac{m}{2} + 1 \le j \le \frac{m}{2}\}$.

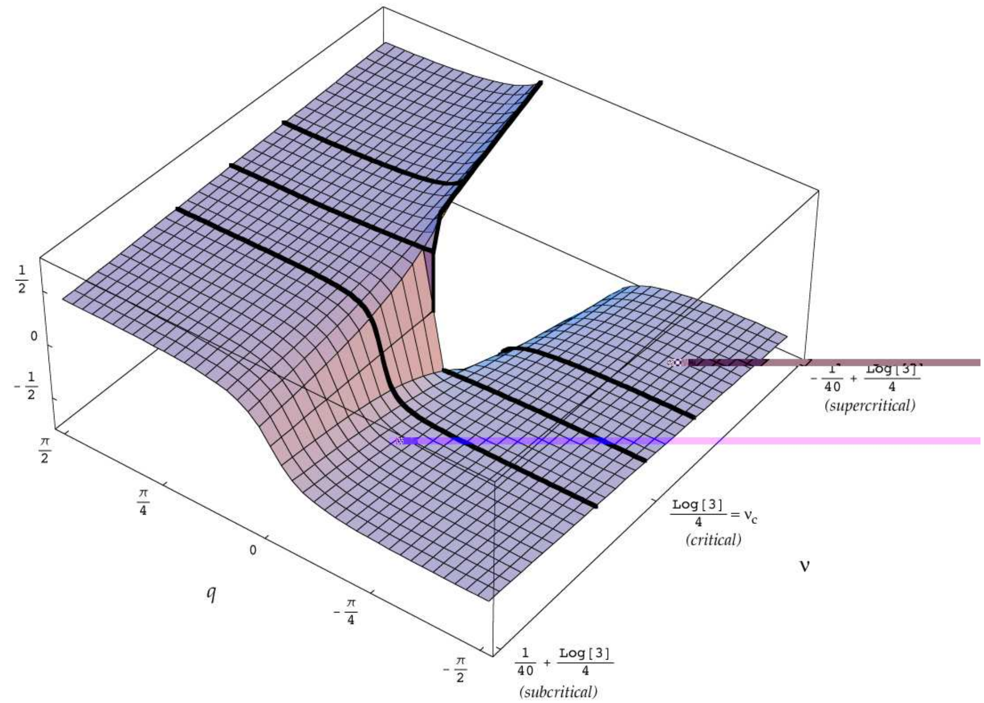

Figure 5: The function Re $d_{\text{even}}(q,\nu)$ for the triangular lattice.

The notation is that of Section 3.

PROOF: We first establish a one-to-one correspondence between summands in

$$\left(\prod_{1\le i\le n}\text{Odd}_{q_i}\right)\text{Sym}_{q_1,q_2,\ldots,q_n}\sum_{\pi\in\text{Pf}_{2n}}(-1)^{l(\pi)}P(q_{\pi(1)},q_{\pi(2)},\ldots,q_{\pi(n)})$$

and in

$$\sum_{\rho\in S_{2n}}(-1)^{l(\rho)}P(q_{\rho(1)},q_{\rho(2)},\ldots,q_{\rho(n)}).$$

Take any permutation ρ in S_{2n}. There exists a unique choice of n permutations $\tau_i\in S_{2n}$, acting trivially on all indices but $2i-1$ and $2i$ such that $\tau_1(\rho(1))<\tau_1(\rho(2))$, $\tau_2(\rho(3))<\tau_2(\rho(4))$, $\ldots$, $\tau_n(\rho(2n-1))<\tau_n(\rho(2n))$. After the pairs have been ordered, there is a single permutation $\sigma\in S_{2n}$ that orders pairs in increasing value of their first elements: $\sigma(\tau_1(\rho(1)))<\sigma(\tau_2(\rho(3)))<\cdots<\sigma(\tau_n(\rho(2n-1)))$. Because the choice of τ_i's amounts to choose one of the two terms in Odd_{q_i} and the choice of σ is one of the terms of the sum $\text{Sym}_{q_1,q_2,\ldots,q_n}$, the one-to-one correspondence stated above follows with $\sigma\tau_1\tau_2\ldots\tau_n\rho=\pi$. In Odd_{q_i}, the term in which q is replaced by $-q$ is multiplied by -1 and the corresponding term in $\sum_{\rho\in S_{2n}}$ should appear with a factor $\prod_i(-1)^{l(\tau_i)}$. There is no alternating sign in the operator Sym. However, because σ permutes pairs, it is an even permutation. Therefore

$(-1)^{l(\pi)}\prod_i(-1)^{l(\tau_i)}=(-1)^{l(\rho)}$ and

$$N_n(q_1,q_2,\ldots,q_n)=\frac{1}{2^n n!}\sum_{1\le k_1<k_2<\cdots<k_{2n}\le m}\ \sum_{\rho\in S_{2n}}(-1)^{l(\rho)}\prod_{1\le j\le n}e^{i(k_{\rho(2j-1)}-k_{\rho(2j)})q_j}. \qquad (43)$$

Note that by the introduction of auxiliary variables $x_{2j-1}=e^{iq_j}$ and $x_{2j}=e^{-iq_j}$ for $1\le j\le n$, the sum over the permutation group S_{2n} becomes simply a determinant:

$$N_n(q_1,q_2,\ldots,q_n)=\frac{1}{2^n n!}\sum_{1\le k_1<k_2<\cdots<k_{2n}\le m}\det\left(x_i^{k_j}\right)_{1\le i,j\le 2n}. \qquad (44)$$

The second step is to transform the sum over ordered $2n$-tuplets $(k_1,k_2,\ldots,k_{2n})$ into a sum over partitions and to introduce the appropriate tools from the theory of symmetric functions. A partition λ is a finite set $\lambda=(\lambda_1,\lambda_2,\ldots)$ of positive non-increasing integers. (See [15] for standard notations and definitions on partitions.) Define the integers $\lambda_i, 1\le i\le 2n$ by $\lambda_i=k_{2n-i+1}-(2n-i+1)$ or $k_j=j+\lambda_{2n+1-j}$. The ordering $1\le k_1<k_2<\cdots<k_{2n}\le m$ is equivalent to $m-2n\ge\lambda_1\ge\lambda_2\ge\ldots\lambda_{2n}\ge 0$. The partial ordering $\mu\subset\lambda$ between partitions stands for $\mu_i\le\lambda_i$, for all i. Finally (M^N) stands for the partition

$$(M^N)=(\underbrace{M,M,\ldots,M}_{N\text{ times}},0,0,\ldots).$$

With this notation, the polynomial N_n can be rewritten as

$$N_n(q_1,q_2,\ldots,q_n)=\frac{1}{2^n n!}\sum_{\lambda\subset((m-2n)^{2n})}\det\left(x_i^{j+\lambda_{2n+1-j}}\right)_{1\le i,j\le 2n}. \qquad (45)$$

One can change the order of rows $(1,2,\ldots,2n)$ to $(2n,2n-1,\ldots,1)$ in the determinant. The number of transpositions has the parity of $(2n)(2n-1)/2=n(2n-1)$ and has therefore the parity of n. Then $\det(x_i^{j+\lambda_{2n+1-j}})_{1\le i,j\le 2n}=(-1)^n\det(x_i^{\lambda_j+2n-j})_{1\le i,j\le 2n}\prod_{1\le j\le 2n}x_j$. In the present case, the value of the x_j's are such that $x_{2j-1}=1/x_{2j}$ and the last product is simply unity. The definition of the Schur function of N variables associated with the partition λ (also to be found in [15]) is $s_\lambda(x_1,x_2,\ldots,x_N)=a_{\lambda+\delta}(x_1,x_2,\ldots,x_N)/a_\delta(x_1,x_2,\ldots,x_N)$ with $a_{\lambda+\delta}(x_1,x_2,\ldots,x_N)=\det(x_i^{\lambda_j+N-j})_{1\le i,j\le N}$ and a_δ is the Vandermonde determinant $a_\delta(x_1,x_2,\ldots,x_N)=\det(x_i^{N-j})_{1\le i,j\le N}=\prod_{1\le i<j\le N}(x_i-x_j)$. The polynomial N_n is then

$$N_n(q_1,q_2,\ldots,q_n)=\frac{(-1)^n}{2^n n!}\prod_{1\le i<j\le N}(x_i-x_j)\sum_{\lambda\subset((m-2n)^{2n})}s_\lambda(x_1,x_2,\ldots,x_{2n}). \qquad (46)$$

This form has the remarkable advantage over previous ones that the above sum over partitions is known to combinatorists. On page 84 of [15] one finds $\sum_{\lambda\subset(M^N)}s_\lambda(x_1,x_2,\ldots,x_N)=D_M/D_0$ where $D_M=\det(x_j^{M+2N-i}-x_j^{i-1})_{1\le i,j\le N}$ and $D_0=\det(x_j^{2N-i}-x_j^{i-1})_{1\le i,j\le N}$. The computation of N_n is then simply that of two determinants.

The third and last step is the computation of D_0 and D_M. Both shares some obvious factors. Note that $M + 2N = m + 2n$ and $N = 2n$ and their forms are

$$D_0 = \begin{vmatrix} x_1^{4n-1} - 1 & x_2^{4n-1} - 1 & \cdots & x_{2n}^{4n-1} - 1 \\ x_1^{4n-2} - x_1 & x_2^{4n-2} - x_2 & \cdots & x_{2n}^{4n-2} - x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{2n} - x_1^{2n-1} & x_2^{2n} - x_2^{2n-1} & \cdots & x_{2n}^{2n} - x_{2n}^{2n-1} \end{vmatrix}$$

and

$$D_M = \begin{vmatrix} x_1^{m+2n-1} - 1 & x_2^{m+2n-1} - 1 & \cdots & x_{2n}^{m+2n-1} - 1 \\ x_1^{m+2n-2} - x_1 & x_2^{m+2n-2} - x_2 & \cdots & x_{2n}^{m+2n-2} - x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{m} - x_1^{2n-1} & x_2^{m} - x_2^{2n-1} & \cdots & x_{2n}^{m} - x_{2n}^{2n-1} \end{vmatrix}.$$

Each element of the j-th row of both D_M and D_0 has an obvious $(x_j - 1)$ factor. (Recall that $m \geq 2n$ and that $m + 2n \geq 2i$ for $1 \leq i \leq 2n$.) Both determinants must contain a factor $\prod_{1 \leq j \leq 2n}(x_j - 1)$. If $x_i = x_j$ for $i \neq j$, these determinants vanish. They must also contain a factor $\prod_{1 \leq i < j \leq 2n}(x_i - x_j)$. Finally, if one does $x_j = 1/x_i$ in the j-th column of D_M, it becomes

$$\begin{aligned} (j\text{-th column})|_{x_j = 1/x_i} &= (x_i^{-m-2n+k} - x_i^{-k+1})_{1 \leq k \leq 2n} && (47) \\ &= -x_i^{-m-2n+1}(x_i^{m+2n-k} - x_i^{k-1})_{1 \leq k \leq 2n} && (48) \\ &= -x_i^{-m-2n+1}(i\text{-th column}) && (49) \end{aligned}$$

and D_M must contain also a factor $\prod_{1 \leq i < j \leq 2n}(x_i x_j - 1)$. A similar computation for D_0 shows that it shares also this factor.

Let us define the *leading* monomial in a polynomial $P \in \mathbb{Q}[x_1, x_2, \ldots, x_{2n}]$ as the one obtained through the following procedure. Among all monomials of P find those that have the largest exponent of x_1. Among the latter find those that have the largest exponent of x_2. And so on till one chooses the one with the largest exponent of x_{2n}. This monomial is the *leading* one. The leading monomial in D_0 is easy to determine. From the above determinantal form, the largest exponent of x_1 is $4n - 1$. Deleting the first column and row, we conclude that the largest exponent of x_2 among the monomials containing x_1^{4n-1} is $4n - 2$. And so on. The leading monomial of D_0 is $\prod_{1 \leq j \leq 2n} x_j^{4n-j}$ and its coefficient is unity. The leading monomial in the factors identified above in D_0

$$d_0 = \prod_{1 \leq j \leq 2n}(x_j - 1) \prod_{1 \leq i < j \leq 2n}(x_i - x_j)(x_i x_j - 1)$$

can be also determined. The first product contributes 1 to the exponent of x_1 in the leading monomial and the second $2(2n - 1)$. This exponent is therefore $(4n - 1)$. Among those monomials containing x_1^{4n-1}, the first product contributes 1 to the exponent of x_2 and the second $(2n - 2) + (2n - 1)$ and the exponent of x_2 in the leading monomial is $4n - 2$. Repeating the argument, it is clear that the leading monomial in the factors above coincide with that of D_0 and its coefficient is also 1. We have thus shown that $D_0 = d_0$ and verified

that D_M has D_0 as factor (but this is a basic fact in the theory of Schur functions). Thus $d_m = D_M/D_0$ is a polynomial $\in \mathbb{Q}[x_1, x_2, \dots, x_{2n}]$. The polynomial N_n has still a new form $N_n(q_1, q_2, \dots, q_n) = \frac{(-1)^n}{2^n n!}\, a_\delta\, d_m$. This simple form has as immediate consequence that N_n vanishes whenever $x_i = x_j$ with $i \neq j$, that is when there exists a pair $1 \leq k, l \leq n$ of distinct integers such that $q_k = q_l$ (i and j have the same parity) or $q_k = -q_l$ (i and j have different parity).

To calculate the value of N_n when all q_i^2 are distinct, let us first remark that some of the factors in a_δ and in D_0 give easily the factors $\cot \frac{1}{2} q_j$ of the proposed answer. Indeed the quotient of the factors $\prod_{1\leq j\leq n}(x_{2j-1} - x_{2j})$ in a_δ with the factors $\prod_{1\leq j\leq 2n}(x_j - 1)$ of D_0 is

$$\frac{\prod_{1\leq j\leq n}(e^{iq_j} - e^{-iq_j})}{\prod_{1\leq j\leq n}(e^{iq_j} - 1)(e^{-iq_j} - 1)} = \left(-\frac{2i}{(2i)^2}\right)^n \prod_{1\leq j\leq n} \frac{\sin q_j}{\sin^2 \frac{1}{2} q_j} = i^n \prod_{1\leq j\leq n} \cot \frac{1}{2} q_j .$$

Let us denote by $\langle i, j\rangle$ pairs of odd integers with $1 \leq i < j < 2n$. Then the residual factors in a_δ, that is those not used in the above quotient, are $\prod_{\langle i,j\rangle}(x_i - x_j)(x_{i+1} - x_j)(x_i - x_{j+1})(x_{i+1} - x_{j+1})$ and those in D_0 are $\prod_{1\leq i<j\leq 2n}(x_i - x_j)(x_i x_j - 1)$ and

$$\begin{aligned} &\frac{1}{i^n \prod_{1\leq j\leq n} \cot \frac{1}{2} q_j} \frac{a_\delta}{D_0} \qquad\qquad (50)\\ &= \frac{1}{\prod_{1\leq j\leq n}(x_{2j-1} - x_{2j})(x_{2j-1}x_{2j} - 1) \prod_{\langle i,j\rangle}(x_i x_j - 1)(x_{i+1}x_j - 1)(x_i x_{j+1} - 1)(x_{i+1}x_{j+1} - 1)} .\end{aligned}$$

The strategy will be to first simplify the factors $(x_{2j-1} - x_{2j})(x_{2j-1}x_{2j} - 1)$ in D_M and then use freely the relation $x_{2j-1} = x_{2j}^{-1}$ in the remaining expression to identify the last factors of (50).

The factors $(x_{2j-1} - x_{2j})(x_{2j-1}x_{2j} - 1)$ occurs in any 2×2 determinant of the elements in the rows $(2k - 1)$ and $(2k)$ and in the lines i and j, $i < j$. If we set $x = x_{2k-1}$ and $y = x_{2k}$, this is

$$d_{ij}(x, y) = \begin{vmatrix} x^{m+2n-i} - x^{i-1} & y^{m+2n-i} - y^{i-1} \\ x^{m+2n-j} - x^{j-1} & y^{m+2n-j} - y^{j-1} \end{vmatrix} .$$

A direct calculation gives

$$(x - y)(xy - 1) \left(x^i y^{j-1} \sum_{k=0}^{j-i-1} (x/y)^k \sum_{l=0}^{m+2n-2-i-j} (xy)^l - x^{m+2n-2-j} y^i \sum_{k=0}^{m+2n-2-i-j} (y/x)^k \sum_{l=0}^{j-i-1} (xy)^l \right) .$$

After simplification with the factors $(x - y)(xy - 1) = (x_{2j-1} - x_{2j})(x_{2j-1}x_{2j} - 1)$ of (50), we can then use the identity $x = y^{-1}$ in the remaining expression $d_{ij}(x, y)/(x - y)(xy - 1) = \omega_{ij}(x)/(x - x^{-1})$ where

$$\omega_{ij}(x) = (m + 2n - 1 - i - j)(x^{j-i} - x^{i-j}) - (j - i)(x^{m+2n-1-i-j} - x^{-(m+2n-1-i-j)}).$$

Define the variables $y_j = x_{2j-1}$ (and $y_j^{-1} = x_{2j}$) for $1 \le j \le n$. The remaining factors of (50) are

$$\prod_{\langle i,j\rangle}(x_ix_j-1)(x_{i+1}x_j-1)(x_ix_{j+1}-1)(x_{i+1}x_{j+1}-1)$$
$$= \prod_{1\le i<j\le n}(y_iy_j-1)(y_i/y_j-1)(y_j/y_i-1)(1/(y_iy_j)-1) \tag{51}$$

and the determinant D_M has the following form in terms of the ω_{ij}:

$$D_M = \frac{1}{\prod_{1\le j\le n}(y_j - y_j^{-1})}(n!\,\mathrm{Sym}_{y_1,y_2,\ldots,y_n}) \sum_{\pi\in \mathrm{Pf}_{2n}} (-1)^{l(\pi)} \prod_{1\le j\le n} \omega_{\pi(2j-1),\pi(2j)}(y_i).$$

(Note that there are $(2n-1)!!$ permutations in Pf_{2n} and that the symmetrization operator gives rise to $n!$ terms out of each summand. The right-hand side contains $(2n-1)!!n! = (2n)!/2^n$ terms. This is the right number as each of the n factors ω's is itself the sum of two terms.) We are now interested in the value of D_M at y_j's such that none of the factors in the denominator is zero. We can therefore evaluate D_M (and the ω's) at $y_j \in Q_m$, that is we can use in D_M the fact that $y_j^m = -1$. (This is the first time since N_n has been expressed in terms of the quotient D_M/D_0 that this is possible.) The ω's are

$$\omega_{ij}(x) = (m+2n-1-i-j)(x^{j-i} - x^{i-j}) + (j-i)(x^{2n-1-i-j} - x^{-(2n-1-i-j)})$$

for x a m-root of -1. We can determine the leading monomial of the polynomial D_M (reduced by replacing all y_j^m by -1) for the variables $y_1, y_2, \ldots, y_n$ taken in that order, y_1 being the first. Because $1 \le i < j \le 2n$, the first term of any ω_{ij} reaches its largest value $(2n-1)$ when $i=1$ and $j=2n$ and the other terms have smaller exponents than this maximum. The leading term in $\omega_{1,2n}(y_1)$ is then my_1^{2n-1}. The range of i and j for $\omega_{ij}(y_2)$ is restricted to $2 \le i < j \le 2n-1$. An analysis similar to the one just done reveals that $i=2, j=2n-1$ are the values to choose and the corresponding ω has leading term my_2^{2n-3}. This process leads to the leading monomial in the above sum over $\pi \in \mathrm{Pf}_{2n}$. It is $\prod_j y_j^{2n-(2j-1)}$. Its coefficient is m^n. The corresponding monomial for D_M is therefore $\prod_j y_j^{2(n-j)}$ with the same coefficient. (Note that the parity of the permutation putting $(1, 2n, 2, 2n-1, \ldots, n-1, n)$ in increasing order is even and that it is Pfaffian.)

Similarly, for the largest exponent of y_1 in (51), the first parenthesis contributes $(n-1)$, the second also $(n-1)$ and the two last ones contribute nothing to the exponent but gives a factor $(-1)^{2n-2}$ to its coefficient. The exponent is then $(2n-2)$. Repeating the argument for the other variables, we find that the leading monomial is the same as for D_M and its coefficient is unity. We must therefore conclude that, upon evaluation of the ω's at m-roots of -1 whose squares are distinct, the quotient of D_M with the residual factors (50) is independent of the q_j chosen and is m^n. The polynomial N_n takes then the value $\frac{1}{n!}(-\frac{im}{2})^n \prod_{1\le j\le n} \cot \frac{1}{2}q_j$ whenever the squares q_j^2 are distinct. $\square$

One has to note that the last calculation that rests upon the use of $y_j \in Q_m$ leads to the wrong answer whenever $y_i = y_j$ or $y_i = y_j^{-1}$ for a given pair of distinct integers i and

j. (The value of N_n at these points was obtained earlier in the proof.) This wrong result is not surprising as both D_M and (51) vanish at these points. One has to cancel out common factors before using the property $y_j \in Q_m$. We have done this exercise only for $m = 4, n = 2$ which is the first non-trivial case. In addition to the $m^n = 4^2$ terms computed above, one gets the following polynomial, after simplification of the common factors and *then* use of $y_j \in Q_m$: $-8 - 4xy + 4x^3y + 4xy^3 - x^3y^3$ which, for $x, y \in Q_m$, is $-m^n(\delta_{xy,1} + \delta_{x/y,1})$. It is obviously the right correction for the theorem to hold.

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